



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2019 – 10:37 AM EDT

PDB ID : 6R4L
Title : Crystal structure of S. cerevisia Niemann-Pick type C protein NCR1
Authors : Winkler, M.B.L.; Kidmose, R.T.; Pedersen, B.P.
Deposited on : 2019-03-22
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

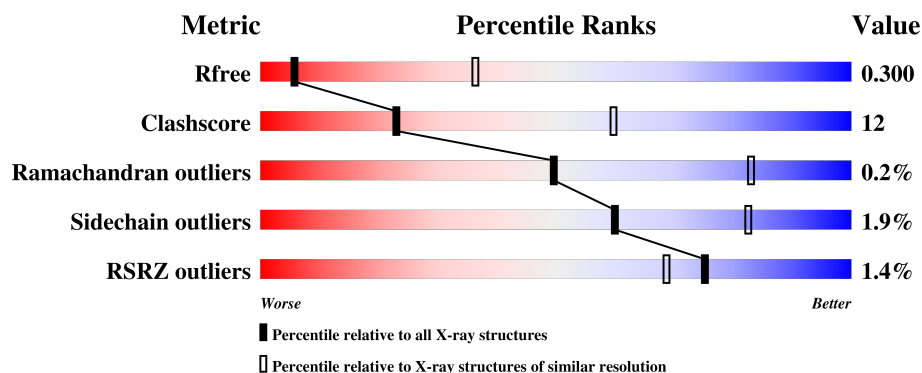
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	111664	1391 (3.60-3.40)
Clashscore	122126	1485 (3.60-3.40)
Ramachandran outliers	120053	1446 (3.60-3.40)
Sidechain outliers	120020	1447 (3.60-3.40)
RSRZ outliers	108989	1303 (3.60-3.40)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	1198	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8894 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 NPC intracellular cholesterol transporter 1-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1096	Total	C	N	O	S	0	0	0
			8759	5706	1390	1606	57			

There are 28 discrepancies between the modelled and reference sequences:

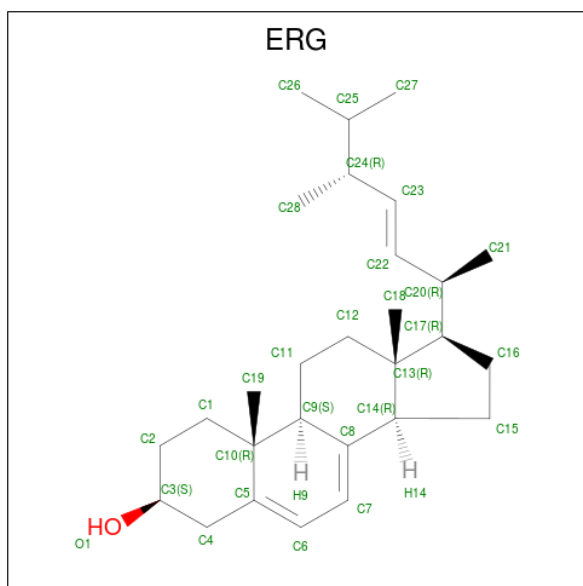
Chain	Residue	Modelled	Actual	Comment	Reference
A	1171	LEU	-	expression tag	UNP Q12200
A	1172	VAL	-	expression tag	UNP Q12200
A	1173	PRO	-	expression tag	UNP Q12200
A	1174	ARG	-	expression tag	UNP Q12200
A	1175	GLY	-	expression tag	UNP Q12200
A	1176	SER	-	expression tag	UNP Q12200
A	1177	GLY	-	expression tag	UNP Q12200
A	1178	GLY	-	expression tag	UNP Q12200
A	1179	GLY	-	expression tag	UNP Q12200
A	1180	GLY	-	expression tag	UNP Q12200
A	1181	SER	-	expression tag	UNP Q12200
A	1182	GLY	-	expression tag	UNP Q12200
A	1183	GLY	-	expression tag	UNP Q12200
A	1184	GLY	-	expression tag	UNP Q12200
A	1185	GLY	-	expression tag	UNP Q12200
A	1186	SER	-	expression tag	UNP Q12200
A	1187	GLY	-	expression tag	UNP Q12200
A	1188	GLY	-	expression tag	UNP Q12200
A	1189	HIS	-	expression tag	UNP Q12200
A	1190	HIS	-	expression tag	UNP Q12200
A	1191	HIS	-	expression tag	UNP Q12200
A	1192	HIS	-	expression tag	UNP Q12200
A	1193	HIS	-	expression tag	UNP Q12200
A	1194	HIS	-	expression tag	UNP Q12200
A	1195	HIS	-	expression tag	UNP Q12200
A	1196	HIS	-	expression tag	UNP Q12200
A	1197	HIS	-	expression tag	UNP Q12200

Continued on next page...

Continued from previous page...

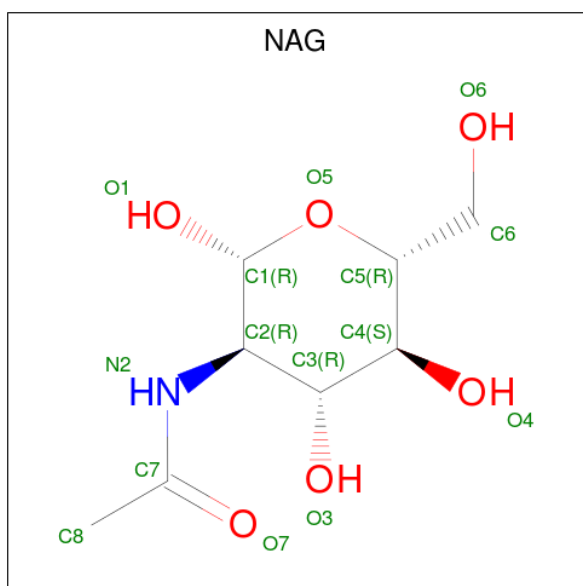
Chain	Residue	Modelled	Actual	Comment	Reference
A	1198	HIS	-	expression tag	UNP Q12200

- Molecule 2 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



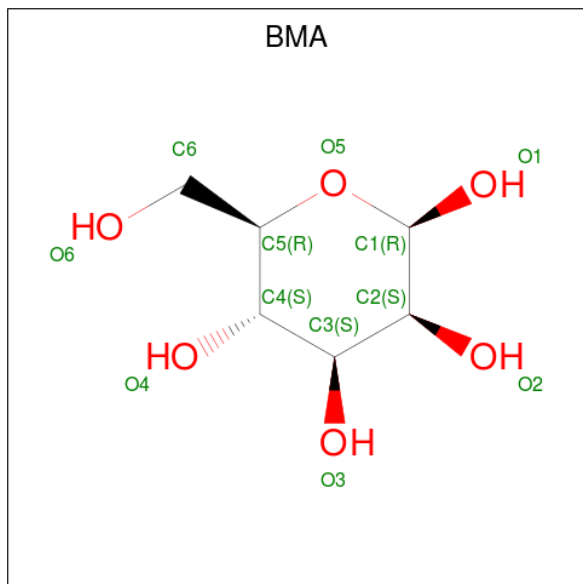
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			29	28	1		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

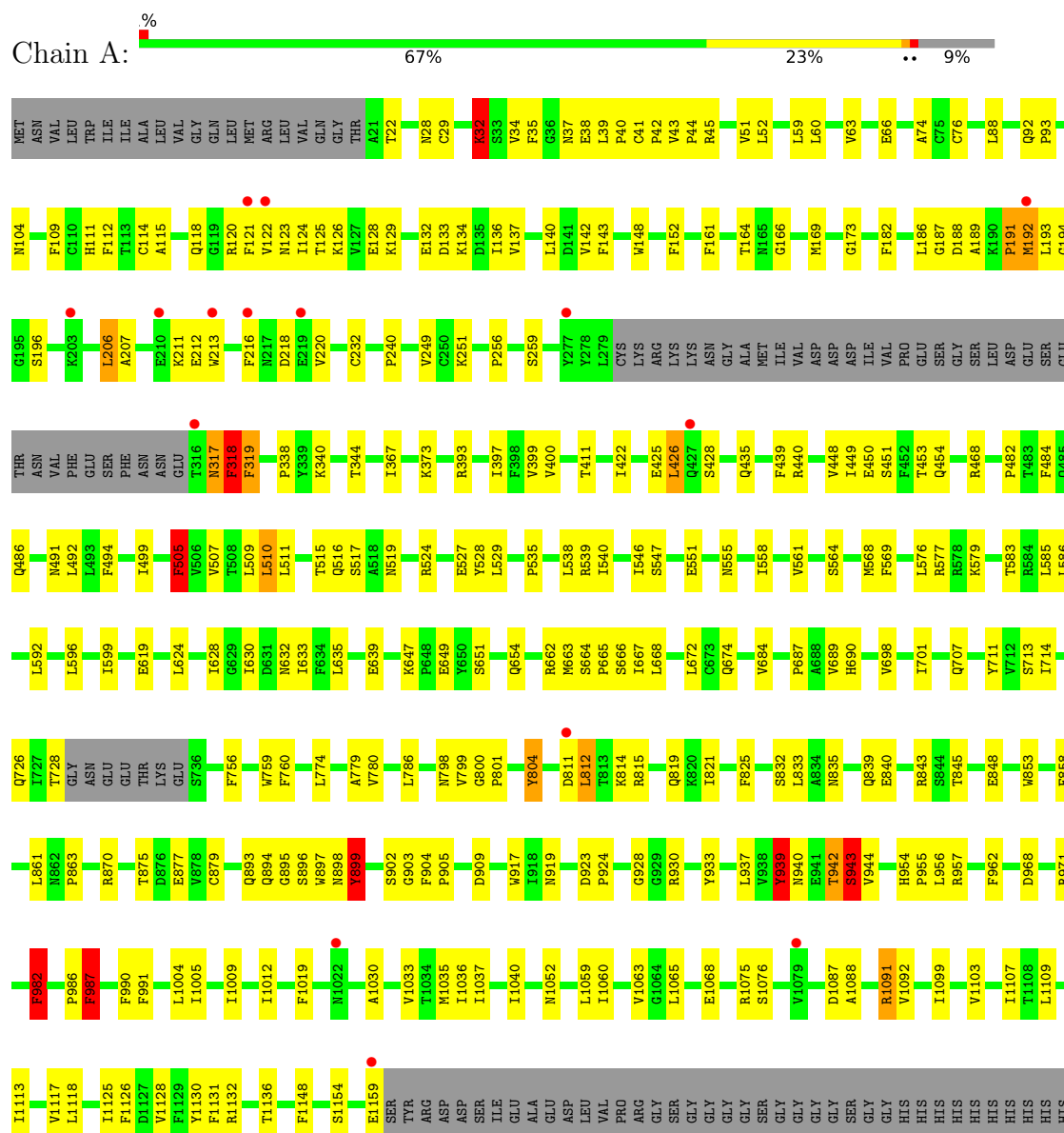


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots

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: NPC intracellular cholesterol transporter 1-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.67Å 90.06Å 161.68Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	49.12 – 3.50 49.12 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.12-3.50) 93.6 (49.12-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.301 0.265 , 0.300	Depositor DCC
R_{free} test set	1209 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	134.5	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERG, NAG, BMA

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	0.53	18/8977 (0.2%)	0.66	15/12185 (0.1%)

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	7

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1159	GLU	CG-CD	8.55	1.64	1.51
1	A	1159	GLU	CD-OE2	8.40	1.34	1.25
1	A	1159	GLU	CD-OE1	8.21	1.34	1.25
1	A	425	GLU	CD-OE1	7.35	1.33	1.25
1	A	899	TYR	CE1-CZ	7.19	1.47	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	899	TYR	CB-CG-CD2	-10.04	114.98	121.00
1	A	982	PHE	CB-CG-CD2	-8.84	114.61	120.80
1	A	505	PHE	CB-CG-CD2	-8.72	114.70	120.80
1	A	943	SER	N-CA-CB	-8.71	97.44	110.50
1	A	987	PHE	CB-CG-CD2	-8.14	115.10	120.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	PRO	Peptide
1	A	318	PHE	Sidechain
1	A	505	PHE	Sidechain
1	A	899	TYR	Sidechain
1	A	939	TYR	Sidechain

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	8759	0	8670	214	0
2	A	29	0	44	5	0
3	A	84	0	74	8	0
4	A	22	0	20	0	0
All	All	8894	0	8808	217	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 12.

The worst 5 of 217 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:212:GLU:HG2	3:A:1208:NAG:H82	1.50	0.93
1:A:517:SER:HB3	3:A:1205:NAG:H83	1.53	0.90
1:A:51:VAL:HG21	1:A:74:ALA:H	1.42	0.85
1:A:426:LEU:HD13	1:A:528:TYR:HB2	1.60	0.83
1:A:451:SER:HB3	1:A:507:VAL:HG23	1.65	0.79

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	1090/1198 (91%)	1004 (92%)	84 (8%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	943	SER
1	A	192	MET

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	981/1064 (92%)	962 (98%)	19 (2%)	60	82

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	PHE
1	A	529	LEU
1	A	943	SER
1	A	426	LEU
1	A	982	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	ASN
1	A	707	GLN
1	A	798	ASN
1	A	835	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	ERG	A	1201	-	31,32,32	0.19	0	45,50,50	0.70	1 (2%)
3	NAG	A	1202	1,3	14,14,15	0.70	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	A	1203	3,4	14,14,15	0.57	0	17,19,21	0.39	0
4	BMA	A	1204	3	11,11,12	0.61	0	15,15,17	1.16	1 (6%)
3	NAG	A	1205	1,3	14,14,15	1.22	1 (7%)	17,19,21	1.11	1 (5%)
3	NAG	A	1206	3,4	14,14,15	0.36	0	17,19,21	0.69	0
4	BMA	A	1207	3	11,11,12	0.96	1 (9%)	15,15,17	1.02	0
3	NAG	A	1208	1	14,14,15	1.28	2 (14%)	17,19,21	0.92	1 (5%)
3	NAG	A	1209	1	14,14,15	1.96	2 (14%)	17,19,21	1.20	2 (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	ERG	A	1201	-	-	4/13/71/71	0/4/4/4
3	NAG	A	1202	1,3	-	3/6/23/26	0/1/1/1
3	NAG	A	1203	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1204	3	-	2/2/19/22	0/1/1/1
3	NAG	A	1205	1,3	-	1/6/23/26	0/1/1/1
3	NAG	A	1206	3,4	-	1/6/23/26	0/1/1/1
4	BMA	A	1207	3	-	0/2/19/22	0/1/1/1
3	NAG	A	1208	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1209	1	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1209	NAG	O5-C1	6.44	1.54	1.43
3	A	1205	NAG	O5-C1	-4.00	1.37	1.43
3	A	1208	NAG	C8-C7	-3.20	1.43	1.50
3	A	1209	NAG	C1-C2	3.10	1.57	1.52
3	A	1208	NAG	O5-C1	-2.84	1.39	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1205	NAG	C3-C4-C5	3.70	116.87	110.23
3	A	1208	NAG	C1-C2-N2	-3.21	105.01	110.49
3	A	1202	NAG	C2-N2-C7	2.90	127.08	122.92
3	A	1209	NAG	C1-O5-C5	2.76	115.95	112.20
4	A	1204	BMA	C1-O5-C5	2.56	115.68	112.20

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

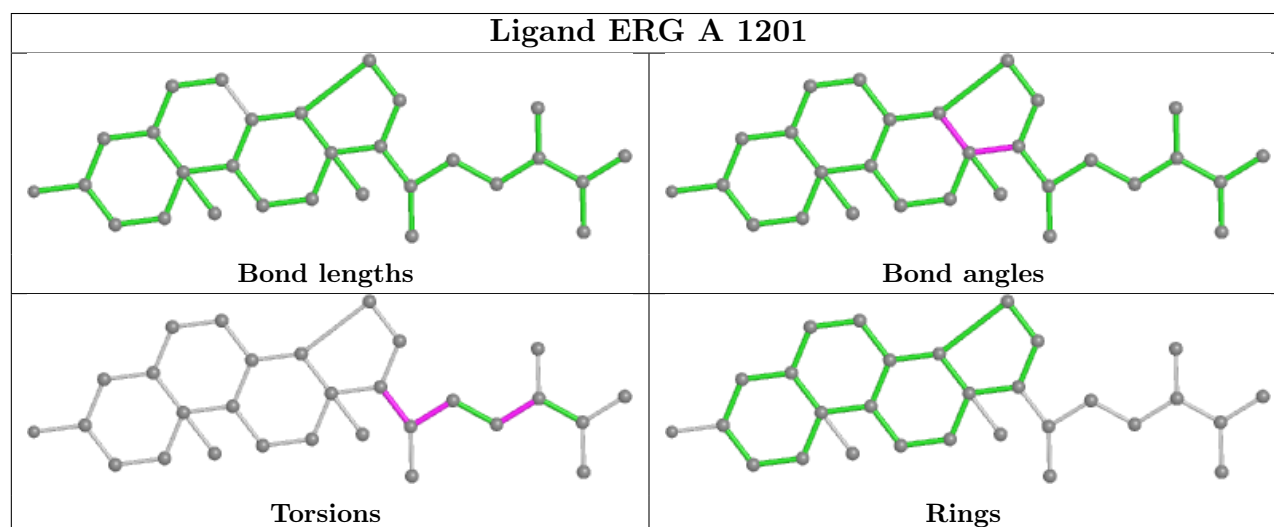
Mol	Chain	Res	Type	Atoms
3	A	1202	NAG	C8-C7-N2-C2
3	A	1202	NAG	O7-C7-N2-C2
3	A	1209	NAG	C8-C7-N2-C2
3	A	1209	NAG	O7-C7-N2-C2
2	A	1201	ERG	C17-C20-C22-C23

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ERG	5	0
3	A	1202	NAG	1	0
3	A	1205	NAG	3	0
3	A	1206	NAG	1	0
3	A	1208	NAG	4	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 [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	1096/1198 (91%)	-0.38	15 (1%) 75 69	74, 156, 215, 362	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	GLU	7.8
1	A	277	TYR	3.7
1	A	210	GLU	3.4
1	A	121	PHE	3.0
1	A	427	GLN	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 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, 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.

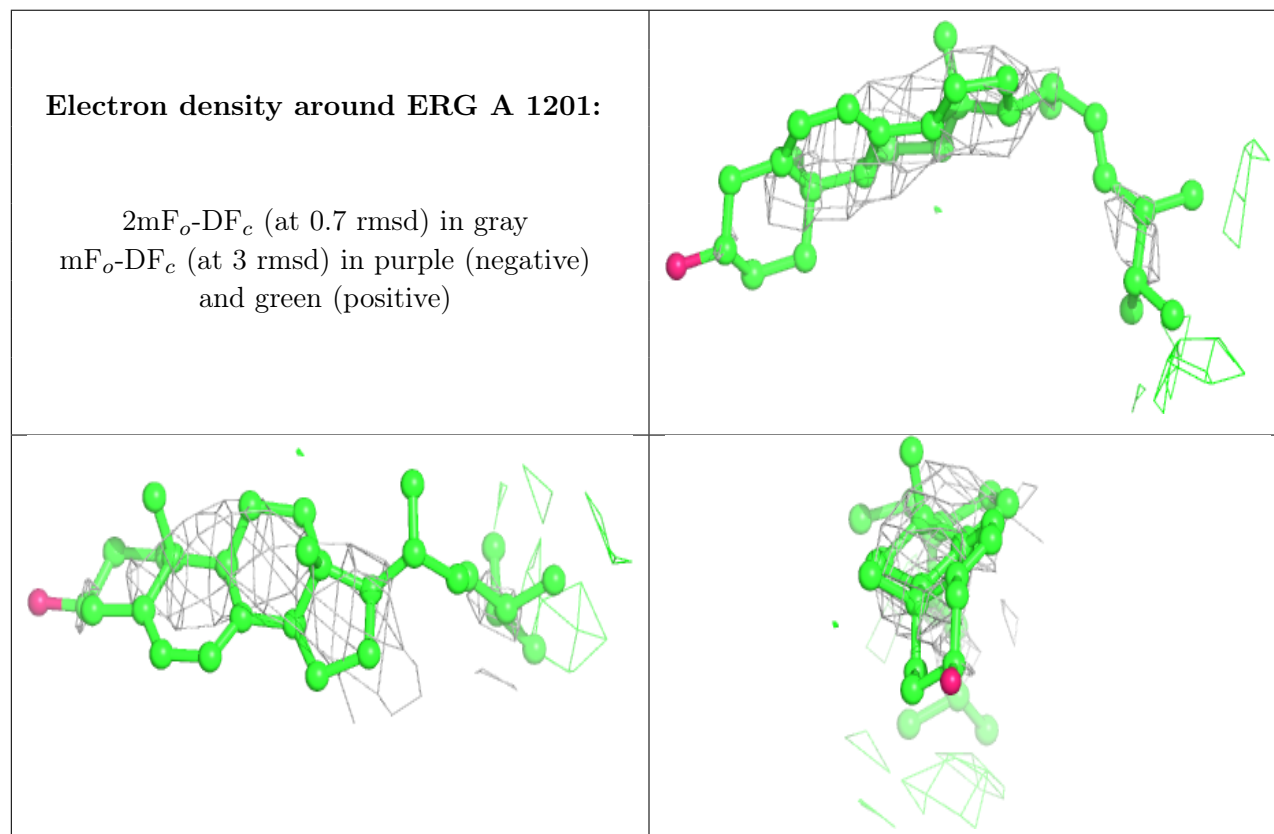
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	A	1207	11/12	0.62	0.22	181,233,243,254	0
3	NAG	A	1208	14/15	0.71	0.26	210,237,265,275	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	1205	14/15	0.74	0.29	240,256,264,268	0
4	BMA	A	1204	11/12	0.74	0.18	184,224,236,239	0
2	ERG	A	1201	29/29	0.79	0.35	142,156,172,175	29
3	NAG	A	1209	14/15	0.84	0.16	186,207,244,247	0
3	NAG	A	1206	14/15	0.85	0.28	207,254,264,266	0
3	NAG	A	1203	14/15	0.88	0.20	191,225,239,249	0
3	NAG	A	1202	14/15	0.91	0.20	194,212,232,243	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.