



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 04:31 pm BST

PDB ID : 9RGS / pdb_00009rgs
Title : Crystal Structure of Rattus norvegicus Enoyl-CoA Hydratase in complex with 3S-hydroxyhexanoyl-CoA
Authors : Dalwani, S.; Wierenga, R.K.
Deposited on : 2025-06-07
Resolution : 1.68 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:

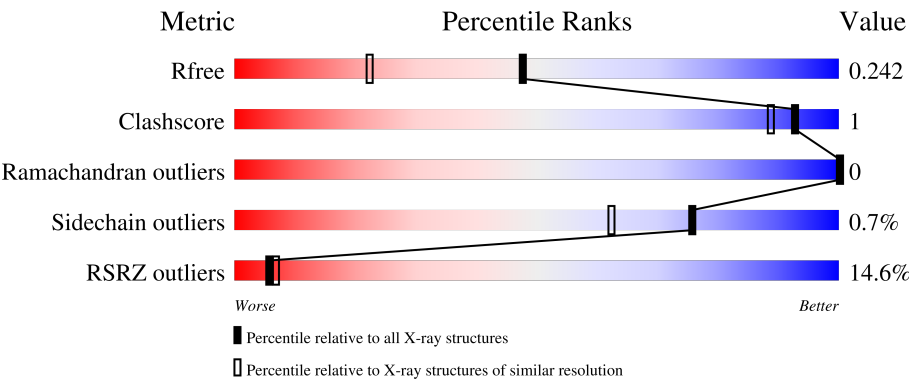
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	290	<div><div>20%</div><div><div></div><div>83%</div><div>•</div><div>12%</div></div></div>
1	D	290	<div><div>12%</div><div><div></div><div>86%</div><div>•</div><div>12%</div></div></div>
1	E	290	<div><div>8%</div><div><div></div><div>84%</div><div>•</div><div>12%</div></div></div>
1	F	290	<div><div>9%</div><div><div></div><div>84%</div><div>•</div><div>12%</div></div></div>
2	B	290	<div><div>12%</div><div><div></div><div>85%</div><div>•</div><div>12%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	C	290	<div><div></div><div>16%</div><div>83%</div><div>•</div><div>12%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12851 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.

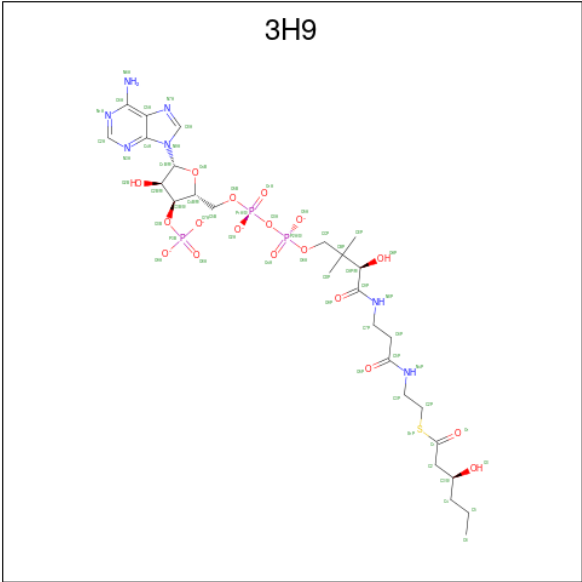
- Molecule 1 is a protein called Enoyl-CoA hydratase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1946	1222	335	376	13			
1	D	256	Total	C	N	O	S	0	0	0
			1939	1215	334	377	13			
1	E	256	Total	C	N	O	S	0	0	0
			1946	1222	335	376	13			
1	F	255	Total	C	N	O	S	0	2	0
			1958	1228	336	380	14			

- Molecule 2 is a protein called Enoyl-CoA hydratase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	1	0
			1938	1220	332	372	14			
2	C	256	Total	C	N	O	S	0	0	0
			1945	1222	335	375	13			

- Molecule 3 is (S)-3-Hydroxyhexanoyl-CoA (CCD ID: 3H9) (formula: $C_{27}H_{42}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		

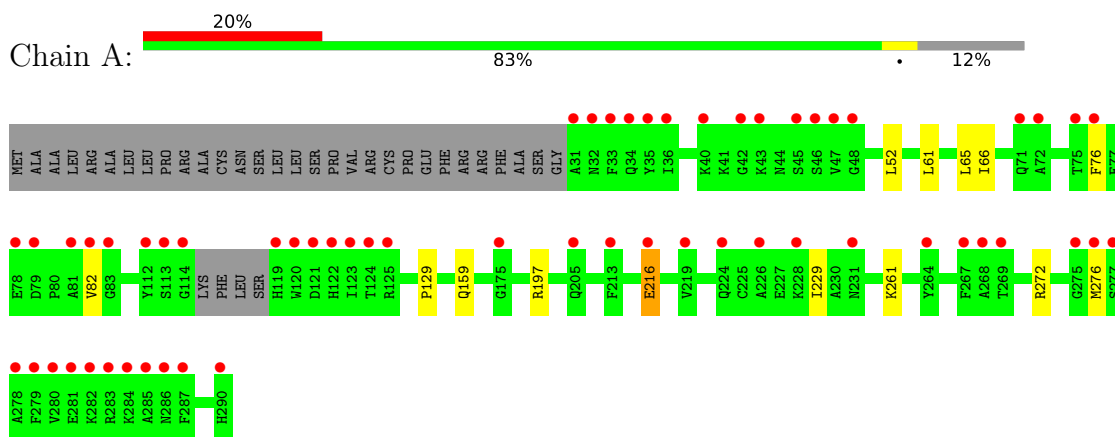
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	167	Total	O	0	0
			167	167		
4	C	120	Total	O	0	0
			120	120		
4	D	139	Total	O	0	0
			139	139		
4	E	166	Total	O	0	0
			166	166		
4	F	164	Total	O	0	0
			164	164		

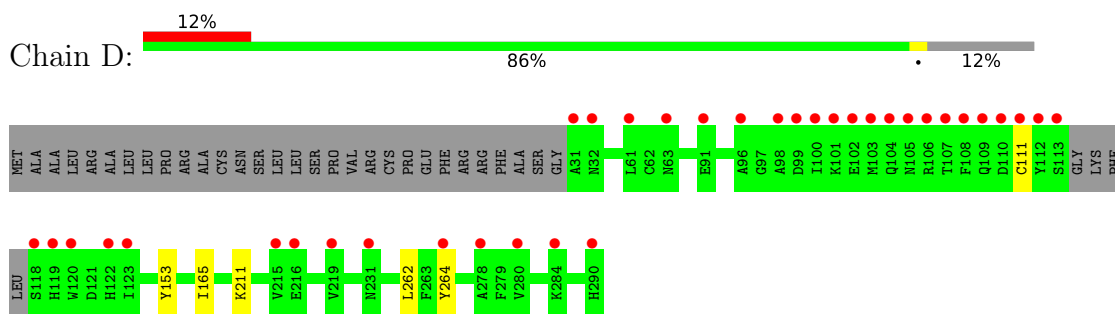
3 Residue-property plots [i](#)

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.

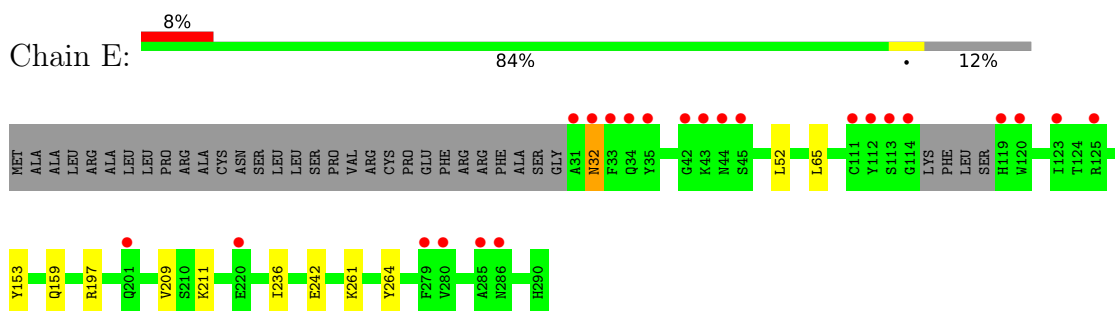
- Molecule 1: Enoyl-CoA hydratase, mitochondrial




- Molecule 1: Enoyl-CoA hydratase, mitochondrial

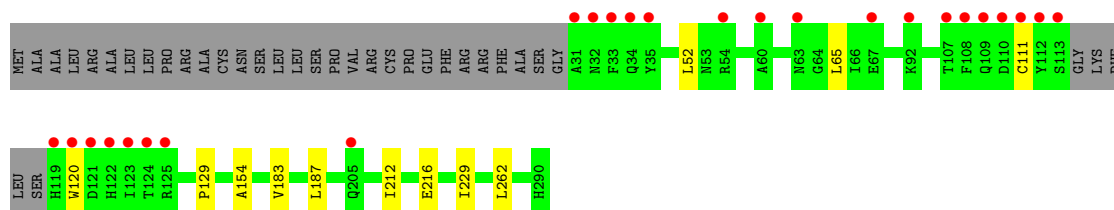


- Molecule 1: Enoyl-CoA hydratase, mitochondrial




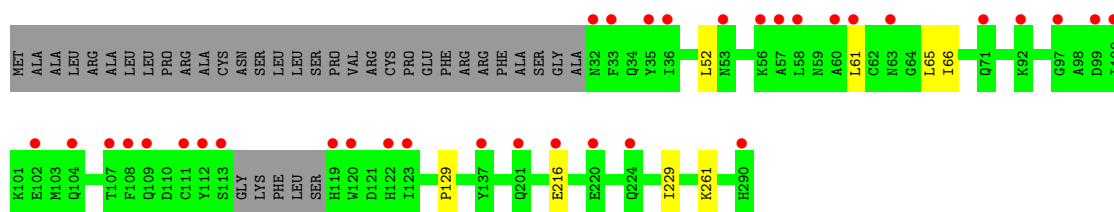
- Molecule 1: Enoyl-CoA hydratase, mitochondrial

Chain F:  9% 84% 12%




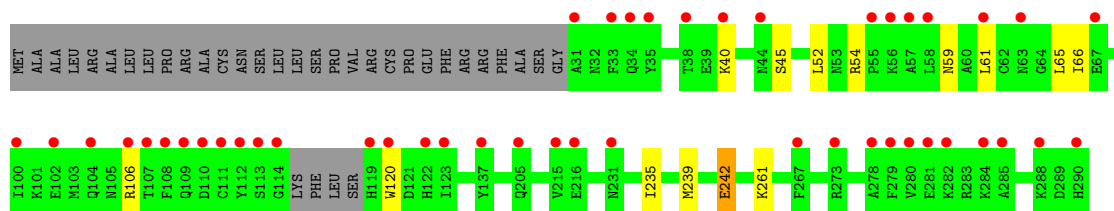
• Molecule 2: Enoyl-CoA hydratase, mitochondrial

Chain B:  12% 85% 12%



• Molecule 2: Enoyl-CoA hydratase, mitochondrial

Chain C:  16% 83% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.08Å 93.69Å 248.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.70 – 1.68 124.34 – 1.68	Depositor EDS
% Data completeness (in resolution range)	55.8 (124.70-1.68) 56.3 (124.34-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.242 0.209 , 0.242	Depositor DCC
R_{free} test set	5600 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12851	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: CSO, 3H9

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	0.43	0/1955	0.90	0/2622
1	D	0.42	0/1946	0.90	0/2609
1	E	0.43	0/1955	0.90	0/2622
1	F	0.42	0/1960	0.89	0/2629
2	B	0.42	0/1958	0.91	0/2627
2	C	0.42	0/1962	0.90	0/2633
All	All	0.42	0/11736	0.90	0/15742

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

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	1946	0	1963	8	0
1	D	1939	0	1956	5	0
1	E	1946	0	1963	8	0
1	F	1958	0	1969	6	0
2	B	1938	0	1960	6	0
2	C	1945	0	1963	9	0
3	A	56	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	42	0	0
3	C	56	0	42	0	0
3	E	56	0	42	0	0
3	F	56	0	42	0	0
4	A	143	0	0	0	0
4	B	167	0	0	1	0
4	C	120	0	0	0	0
4	D	139	0	0	0	0
4	E	166	0	0	0	0
4	F	164	0	0	0	0
All	All	12851	0	11984	35	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 1.

All (35) 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)
2:C:52:LEU:HD22	2:C:65:LEU:HD21	1.82	0.62
1:F:52:LEU:HD22	1:F:65:LEU:HD21	1.83	0.61
2:C:54:ARG:H	2:C:59:ASN:ND2	1.99	0.60
2:B:129:PRO:HG2	2:B:229:ILE:HG21	1.83	0.60
2:C:54:ARG:H	2:C:59:ASN:HD21	1.51	0.57
2:B:52:LEU:HD22	2:B:65:LEU:HD21	1.89	0.54
1:F:129:PRO:HG2	1:F:229:ILE:HG21	1.91	0.53
1:D:111:CYS:HB3	1:E:264:TYR:CD1	2.45	0.52
2:C:242:GLU:HG2	1:E:261:LYS:HE2	1.94	0.50
1:A:216:GLU:H	1:A:216:GLU:CD	2.19	0.50
2:B:216:GLU:HB2	4:B:457:HOH:O	2.12	0.49
2:C:40:LYS:HE2	2:C:45:SER:HB3	1.93	0.49
1:E:153:TYR:CD1	1:E:211:LYS:HB2	2.48	0.49
2:C:261:LYS:HE2	1:E:242:GLU:HG2	1.94	0.48
2:B:261:LYS:HD3	1:F:262:LEU:HD21	1.96	0.47
1:A:52:LEU:HD22	1:A:65:LEU:HD21	1.97	0.47
1:D:264:TYR:CD1	1:F:111:CYS:HB3	2.50	0.46
2:C:61:LEU:HB3	2:C:66:ILE:HD11	1.99	0.44
1:E:159:GLN:NE2	1:E:197:ARG:HE	2.14	0.44
2:C:40:LYS:HB3	2:C:45:SER:HB3	2.00	0.44
2:C:235:ILE:HG12	2:C:239:MET:HE3	2.00	0.44
1:F:183:VAL:HB	1:F:187:LEU:HD23	2.00	0.43
1:E:32:ASN:HD22	1:E:32:ASN:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HB3	1:A:66:ILE:HD11	2.01	0.42
1:E:52:LEU:HD22	1:E:65:LEU:HD21	2.01	0.42
2:B:61:LEU:HB3	2:B:66:ILE:HD11	2.01	0.42
1:D:153:TYR:CD1	1:D:211:LYS:HB2	2.54	0.42
1:A:272:ARG:HH11	1:A:276:MET:HG3	1.85	0.42
1:A:129:PRO:HG2	1:A:229:ILE:HG21	2.01	0.41
1:A:261:LYS:HD3	1:D:262:LEU:HD21	2.03	0.41
2:B:129:PRO:HG2	2:B:229:ILE:CG2	2.49	0.41
1:F:154:ALA:O	1:F:212:ILE:HA	2.21	0.41
1:D:165:ILE:HD12	1:E:236:ILE:HG22	2.03	0.41
1:A:76:PHE:HD1	1:A:82:VAL:HG21	1.86	0.40
1:A:159:GLN:NE2	1:A:197:ARG:HE	2.20	0.40

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	250/290 (86%)	249 (100%)	1 (0%)	0	100	100
1	D	250/290 (86%)	248 (99%)	2 (1%)	0	100	100
1	E	250/290 (86%)	248 (99%)	2 (1%)	0	100	100
1	F	250/290 (86%)	244 (98%)	6 (2%)	0	100	100
2	B	250/290 (86%)	247 (99%)	3 (1%)	0	100	100
2	C	251/290 (87%)	244 (97%)	7 (3%)	0	100	100
All	All	1501/1740 (86%)	1480 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	199/227 (88%)	198 (100%)	1 (0%)	81	72
1	D	199/227 (88%)	199 (100%)	0	100	100
1	E	199/227 (88%)	197 (99%)	2 (1%)	68	52
1	F	200/227 (88%)	198 (99%)	2 (1%)	68	52
2	B	200/228 (88%)	200 (100%)	0	100	100
2	C	200/228 (88%)	197 (98%)	3 (2%)	57	34
All	All	1197/1364 (88%)	1189 (99%)	8 (1%)	76	62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
2	C	106	ARG
2	C	120	TRP
2	C	242	GLU
1	E	32	ASN
1	E	209	VAL
1	F	120	TRP
1	F	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	162	GLN
1	A	224	GLN
2	B	34	GLN
2	B	51	GLN
2	B	71	GLN
2	B	159	GLN
2	B	162	GLN
2	B	201	GLN

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Mol	Chain	Res	Type
2	B	286	ASN
2	C	51	GLN
2	C	59	ASN
2	C	159	GLN
2	C	205	GLN
2	C	224	GLN
1	D	51	GLN
1	D	122	HIS
1	D	159	GLN
1	E	32	ASN
1	E	34	GLN
1	E	159	GLN
1	E	162	GLN
1	E	224	GLN
1	F	51	GLN
1	F	122	HIS
1	F	159	GLN
1	F	201	GLN
1	F	205	GLN
1	F	224	GLN
1	F	286	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	E	62	1	3,6,7	0.75	0	0,6,8	-	-
1	CSO	E	225	1	3,6,7	0.69	0	0,6,8	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	D	62	1	3,6,7	0.72	0	0,6,8	-	-
2	CSO	C	225	2	3,6,7	0.75	0	0,6,8	-	-
2	CSO	B	225	2	3,6,7	0.80	0	0,6,8	-	-
1	CSO	A	62	1	3,6,7	0.66	0	0,6,8	-	-
1	CSO	F	225[B]	1	3,6,7	0.74	0	0,6,8	-	-
1	CSO	D	225	1	3,6,7	0.73	0	0,6,8	-	-
1	CSO	A	225	1	3,6,7	0.73	0	0,6,8	-	-
1	CSO	F	225[A]	1	3,6,7	0.78	0	0,6,8	-	-
1	CSO	F	62	1	3,6,7	0.74	0	0,6,8	-	-

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
1	CSO	E	62	1	-	0/1/5/7	-
1	CSO	E	225	1	-	0/1/5/7	-
1	CSO	D	62	1	-	0/1/5/7	-
2	CSO	C	225	2	-	0/1/5/7	-
2	CSO	B	225	2	-	0/1/5/7	-
1	CSO	A	62	1	-	0/1/5/7	-
1	CSO	F	225[B]	1	-	0/1/5/7	-
1	CSO	D	225	1	-	0/1/5/7	-
1	CSO	A	225	1	-	0/1/5/7	-
1	CSO	F	225[A]	1	-	0/1/5/7	-
1	CSO	F	62	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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	3H9	E	301	-	52,58,58	0.45	0	73,85,85	0.54	0
3	3H9	F	301	-	52,58,58	0.46	0	73,85,85	0.61	2 (2%)
3	3H9	A	301	-	52,58,58	0.44	0	73,85,85	0.53	0
3	3H9	B	301	-	52,58,58	0.47	0	73,85,85	0.63	2 (2%)
3	3H9	C	301	-	52,58,58	0.48	1 (1%)	73,85,85	0.63	2 (2%)

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	3H9	E	301	-	-	8/58/74/74	0/3/3/3
3	3H9	F	301	-	-	3/58/74/74	0/3/3/3
3	3H9	A	301	-	-	6/58/74/74	0/3/3/3
3	3H9	B	301	-	-	2/58/74/74	0/3/3/3
3	3H9	C	301	-	-	3/58/74/74	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	3H9	P3B-O3B	2.02	1.63	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	3H9	O3B-C3B-C4B	3.07	121.20	110.08
3	C	301	3H9	O3B-C3B-C2B	2.97	122.43	111.68
3	F	301	3H9	O3B-C3B-C2B	2.76	121.69	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	3H9	O3B-C3B-C2B	2.70	121.45	111.68
3	C	301	3H9	O3B-C3B-C4B	2.37	118.64	110.08
3	F	301	3H9	O3B-C3B-C4B	2.14	117.83	110.08

There are no chirality outliers.

All (22) torsion outliers are listed below:

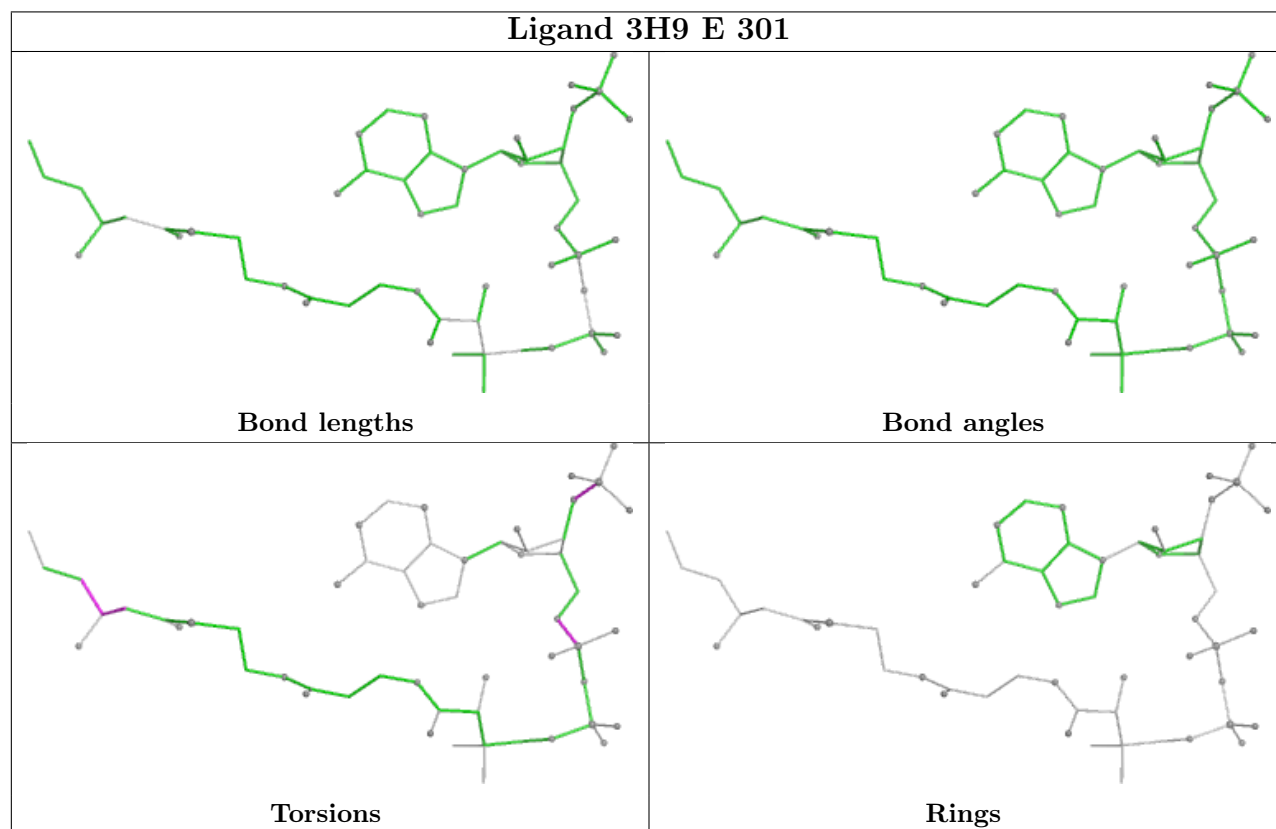
Mol	Chain	Res	Type	Atoms
3	A	301	3H9	C5B-O5B-P1A-O2A
3	A	301	3H9	C3B-O3B-P3B-O7A
3	E	301	3H9	C1-C2-C3-O3
3	E	301	3H9	C1-C2-C3-C4
3	E	301	3H9	C5B-O5B-P1A-O2A
3	F	301	3H9	C1-C2-C3-O3
3	F	301	3H9	C1-C2-C3-C4
3	C	301	3H9	C2B-C3B-O3B-P3B
3	A	301	3H9	C5B-O5B-P1A-O3A
3	E	301	3H9	C5B-O5B-P1A-O3A
3	E	301	3H9	C3B-O3B-P3B-O7A
3	A	301	3H9	C1-C2-C3-C4
3	C	301	3H9	C1-C2-C3-C4
3	E	301	3H9	O3-C3-C4-C5
3	F	301	3H9	C2B-C3B-O3B-P3B
3	A	301	3H9	C1-C2-C3-O3
3	B	301	3H9	C1-C2-C3-O3
3	C	301	3H9	C1-C2-C3-O3
3	E	301	3H9	C3B-O3B-P3B-O9A
3	A	301	3H9	C5B-O5B-P1A-O1A
3	B	301	3H9	C1-C2-C3-C4
3	E	301	3H9	C5B-O5B-P1A-O1A

There are no ring outliers.

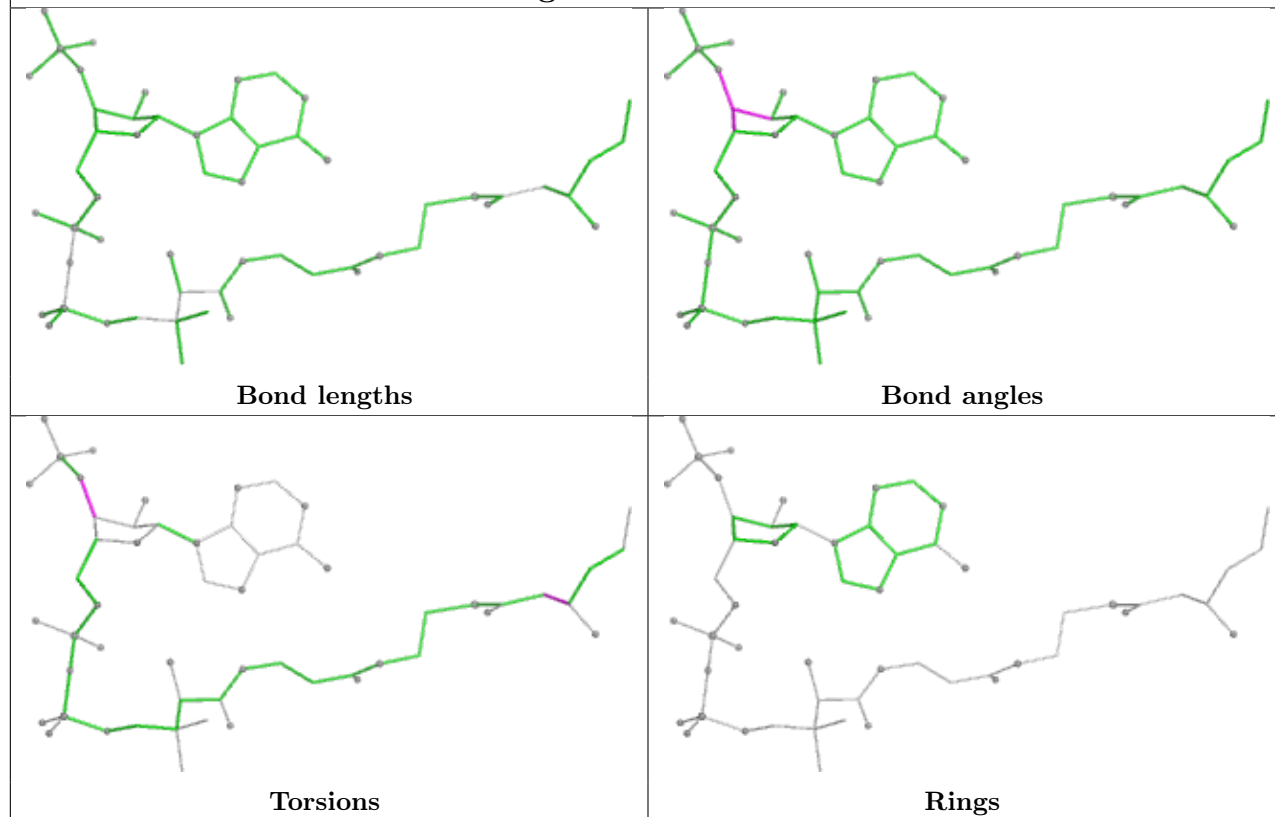
No monomer is involved in short contacts.

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

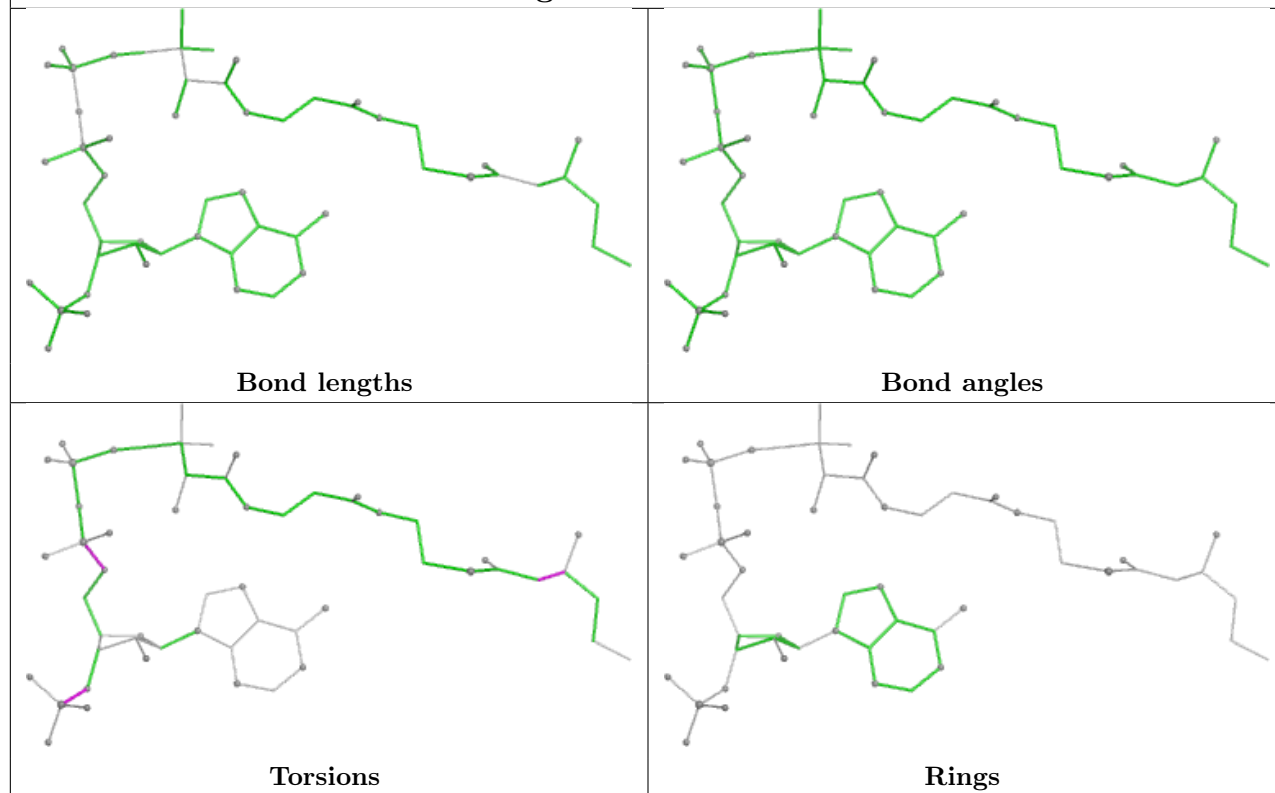
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



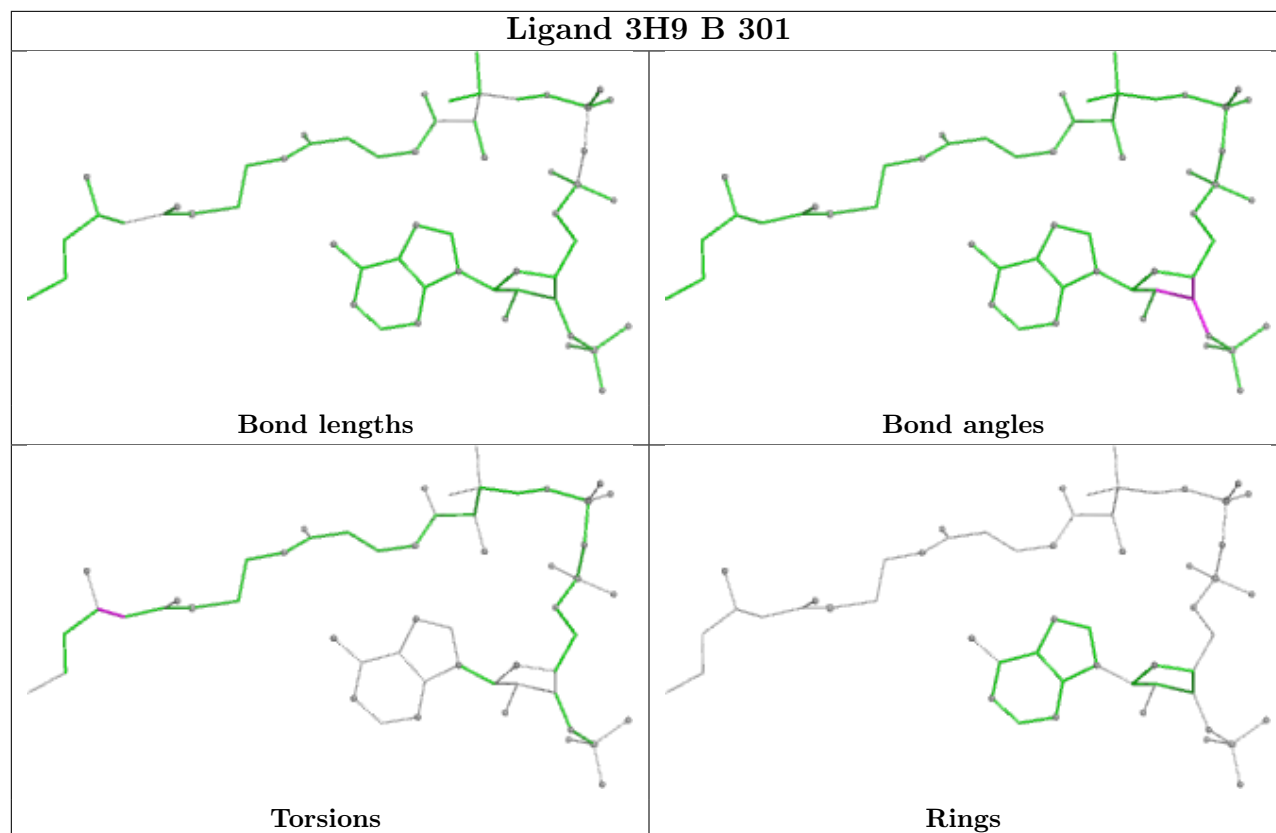
Ligand 3H9 F 301



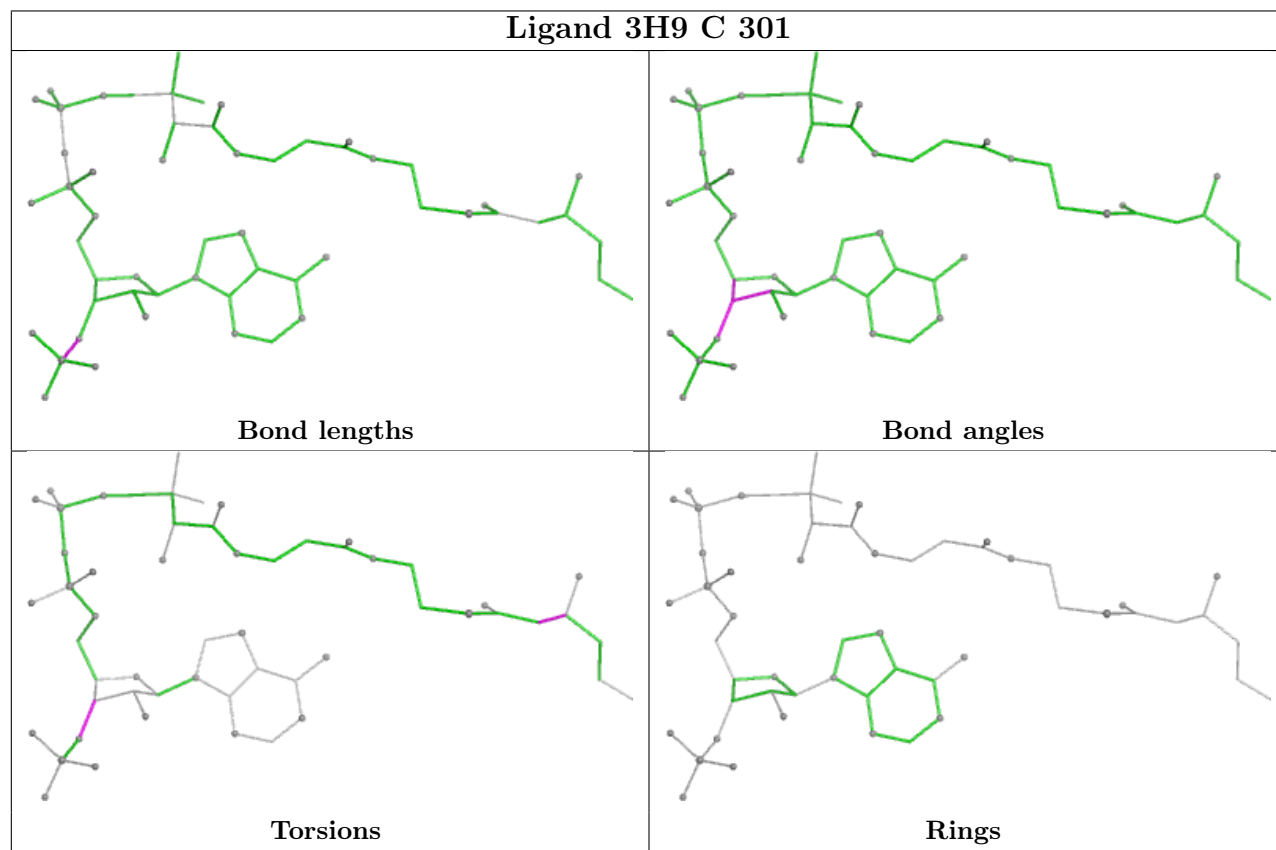
Ligand 3H9 A 301



Ligand 3H9 B 301



Ligand 3H9 C 301



5.7 Other polymers

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 ⓘ

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, 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	254/290 (87%)	0.97	59 (23%) 2 2	14, 27, 53, 73	0
1	D	254/290 (87%)	0.81	36 (14%) 6 7	14, 25, 71, 89	0
1	E	254/290 (87%)	0.54	23 (9%) 15 17	12, 23, 44, 68	0
1	F	253/290 (87%)	0.55	25 (9%) 13 15	8, 21, 52, 76	1 (0%)
2	B	253/290 (87%)	0.69	34 (13%) 7 9	10, 23, 52, 75	1 (0%)
2	C	255/290 (87%)	1.20	46 (18%) 3 4	14, 32, 61, 87	0
All	All	1523/1740 (87%)	0.80	223 (14%) 6 7	8, 25, 54, 89	2 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	31	ALA	8.0
2	C	112	TYR	7.7
1	D	112	TYR	7.4
1	E	31	ALA	7.3
1	D	120	TRP	7.1
2	C	108	PHE	6.9
1	A	31	ALA	6.8
1	E	114	GLY	6.7
2	B	119	HIS	6.1
2	B	120	TRP	5.8
1	F	112	TYR	5.7
2	C	31	ALA	5.5
1	D	107	THR	5.5
1	A	120	TRP	5.5
1	D	31	ALA	5.4
2	C	120	TRP	5.4
1	F	111	CYS	5.3
1	D	108	PHE	5.2
2	C	119	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
2	C	114	GLY	5.1
1	A	280	VAL	5.0
1	D	111	CYS	4.9
1	F	120	TRP	4.9
2	C	111	CYS	4.9
1	A	119	HIS	4.8
2	B	112	TYR	4.7
1	F	119	HIS	4.5
1	D	113	SER	4.5
1	F	108	PHE	4.4
1	E	34	GLN	4.3
2	C	107	THR	4.2
1	F	122	HIS	4.1
1	F	123	ILE	4.1
1	A	114	GLY	4.0
1	D	101	LYS	3.9
1	D	103	MET	3.9
1	A	82	VAL	3.8
1	A	33	PHE	3.8
1	D	118	SER	3.8
1	D	100	ILE	3.8
1	E	119	HIS	3.8
1	E	113	SER	3.6
1	E	120	TRP	3.5
2	B	123	ILE	3.5
1	A	113	SER	3.5
1	A	43	LYS	3.5
1	F	109	GLN	3.5
1	A	34	GLN	3.4
1	D	123	ILE	3.4
2	C	122	HIS	3.4
1	D	119	HIS	3.4
2	C	56	LYS	3.4
1	F	113	SER	3.4
2	C	123	ILE	3.3
1	A	279	PHE	3.3
1	E	44	ASN	3.3
1	F	32	ASN	3.3
2	C	35	TYR	3.3
1	E	201	GLN	3.3
2	B	32	ASN	3.3
2	C	284	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	35	TYR	3.2
1	D	32	ASN	3.2
2	C	279	PHE	3.2
1	F	107	THR	3.2
2	B	58	LEU	3.2
1	D	110	ASP	3.1
1	D	104	GLN	3.1
1	D	264	TYR	3.1
1	F	35	TYR	3.1
2	C	109	GLN	3.1
2	B	63	ASN	3.1
1	A	79	ASP	3.1
1	A	32	ASN	3.1
1	A	226	ALA	3.1
1	A	285	ALA	3.1
1	A	264	TYR	3.0
1	A	290	HIS	3.0
1	F	33	PHE	3.0
1	A	269	THR	3.0
2	C	34	GLN	3.0
1	F	110	ASP	3.0
1	A	123	ILE	3.0
1	E	286	ASN	3.0
1	E	33	PHE	3.0
1	E	43	LYS	2.9
1	E	112	TYR	2.9
2	C	273	ARG	2.9
2	C	57	ALA	2.9
1	E	32	ASN	2.9
2	C	290	HIS	2.9
2	C	280	VAL	2.9
2	C	106	ARG	2.9
1	D	102	GLU	2.9
2	B	109	GLN	2.8
2	C	33	PHE	2.8
1	A	219	VAL	2.8
1	D	280	VAL	2.8
2	B	122	HIS	2.8
2	C	215	VAL	2.7
1	A	122	HIS	2.7
1	D	109	GLN	2.7
2	B	108	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	124	THR	2.7
1	A	268	ALA	2.7
2	C	231	ASN	2.7
1	A	278	ALA	2.7
2	B	60	ALA	2.7
1	D	106	ARG	2.6
1	D	290	HIS	2.6
1	D	231	ASN	2.6
1	A	112	TYR	2.6
1	F	34	GLN	2.6
2	B	57	ALA	2.6
2	C	113	SER	2.6
1	A	76	PHE	2.6
2	B	33	PHE	2.6
1	A	224	GLN	2.6
1	E	123	ILE	2.6
1	A	276	MET	2.6
1	E	42	GLY	2.6
1	F	121	ASP	2.6
1	D	105	ASN	2.6
1	F	60	ALA	2.6
1	F	125	ARG	2.6
2	B	56	LYS	2.5
1	A	78	GLU	2.5
1	A	40	LYS	2.5
1	D	99	ASP	2.5
2	C	104	GLN	2.5
2	C	205	GLN	2.5
2	C	278	ALA	2.5
2	C	102	GLU	2.5
2	B	113	SER	2.5
1	E	35	TYR	2.5
1	A	47	VAL	2.5
2	B	97	GLY	2.5
1	A	213	PHE	2.4
1	A	282	LYS	2.4
1	A	284	LYS	2.4
1	A	287	PHE	2.4
1	D	122	HIS	2.4
1	E	279	PHE	2.4
2	C	285	ALA	2.4
1	A	231	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	75	THR	2.4
2	B	107	THR	2.4
2	C	100	ILE	2.4
1	A	283	ARG	2.4
1	A	275	GLY	2.4
1	A	205	GLN	2.4
1	D	63	ASN	2.4
2	B	92	LYS	2.4
2	B	71	GLN	2.3
2	B	224	GLN	2.3
2	C	55	PRO	2.3
2	B	102	GLU	2.3
2	B	216	GLU	2.3
1	D	278	ALA	2.3
2	C	38	THR	2.3
1	A	267	PHE	2.3
1	A	35	TYR	2.3
1	E	280	VAL	2.3
1	A	281	GLU	2.3
1	A	125	ARG	2.3
1	F	92	LYS	2.3
2	C	282	LYS	2.3
1	E	285	ALA	2.3
1	D	61	LEU	2.3
2	B	61	LEU	2.3
2	C	137	TYR	2.3
1	A	45	SER	2.3
1	A	48	GLY	2.3
2	B	201	GLN	2.3
2	C	58	LEU	2.3
1	F	63	ASN	2.3
1	A	277	SER	2.3
1	A	216	GLU	2.2
1	E	111	CYS	2.2
2	B	111	CYS	2.2
2	B	53	ASN	2.2
1	A	121	ASP	2.2
2	C	110	ASP	2.2
2	B	220	GLU	2.2
1	A	124	THR	2.2
1	A	46	SER	2.2
1	E	125	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	63	ASN	2.2
1	A	72	ALA	2.2
2	C	216	GLU	2.2
2	C	61	LEU	2.2
1	A	228	LYS	2.2
1	A	286	ASN	2.2
1	A	81	ALA	2.1
2	C	288	LYS	2.1
1	F	205	GLN	2.1
1	A	36	ILE	2.1
2	B	137	TYR	2.1
1	F	54	ARG	2.1
1	D	98	ALA	2.1
1	A	175	GLY	2.1
1	A	71	GLN	2.1
1	E	45	SER	2.1
1	E	220	GLU	2.1
2	B	36	ILE	2.1
2	B	100	ILE	2.1
1	D	215	VAL	2.1
2	C	44	ASN	2.1
1	F	67	GLU	2.1
2	B	99	ASP	2.1
2	B	290	HIS	2.1
1	D	284	LYS	2.1
1	A	42	GLY	2.0
2	C	40	LYS	2.0
1	D	91	GLU	2.0
1	D	216	GLU	2.0
2	C	67	GLU	2.0
2	C	281	GLU	2.0
1	A	83	GLY	2.0
2	B	104	GLN	2.0
2	C	267	PHE	2.0
1	D	96	ALA	2.0
1	D	219	VAL	2.0

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

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(\AA^2)	Q<0.9
1	CSO	D	225	7/8	0.78	0.13	26,29,33,36	0
1	CSO	E	225	7/8	0.78	0.15	28,29,35,37	0
1	CSO	A	225	7/8	0.83	0.14	40,42,47,48	0
2	CSO	C	225	7/8	0.84	0.12	37,38,42,44	0
2	CSO	B	225	7/8	0.89	0.11	23,25,30,31	0
1	CSO	D	62	7/8	0.91	0.10	34,35,37,37	0
1	CSO	F	225[A]	7/8	0.91	0.12	21,21,22,23	7
1	CSO	F	225[B]	7/8	0.91	0.12	23,23,24,24	7
1	CSO	F	62	7/8	0.92	0.10	35,36,38,40	0
1	CSO	A	62	7/8	0.94	0.09	26,28,29,30	0
1	CSO	E	62	7/8	0.94	0.08	21,23,24,25	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

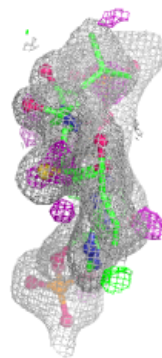
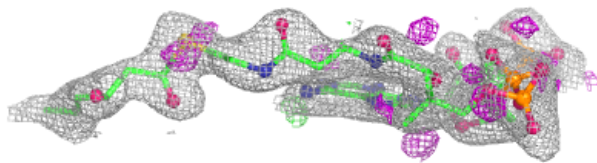
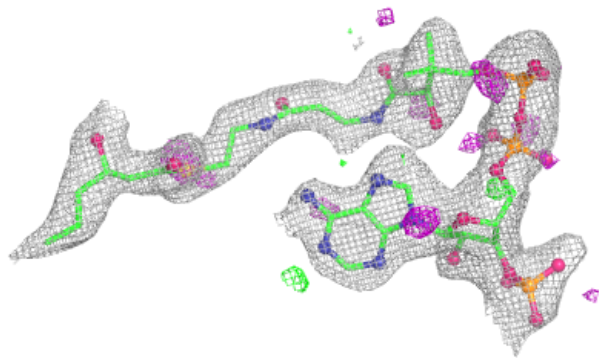
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3H9	B	301	56/56	0.85	0.14	28,49,57,58	0
3	3H9	F	301	56/56	0.87	0.12	28,37,49,50	0
3	3H9	C	301	56/56	0.88	0.12	33,45,48,49	0
3	3H9	E	301	56/56	0.96	0.06	15,19,26,27	0
3	3H9	A	301	56/56	0.96	0.07	17,21,27,28	0

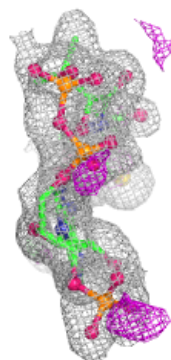
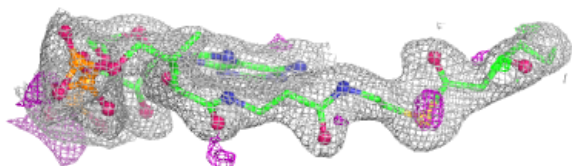
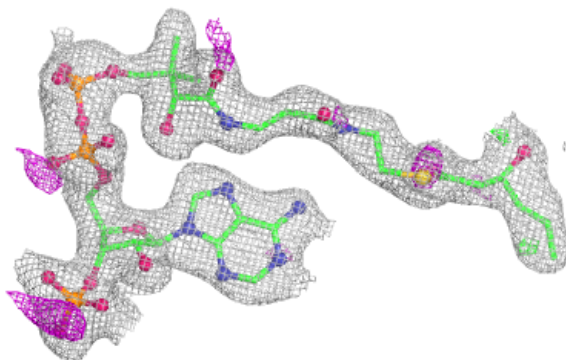
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3H9 B 301:

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

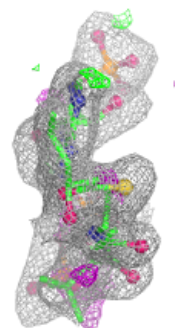
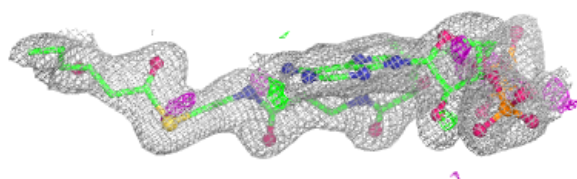
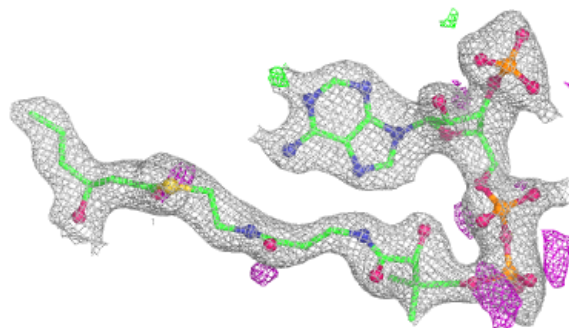
**Electron density around 3H9 F 301:**

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

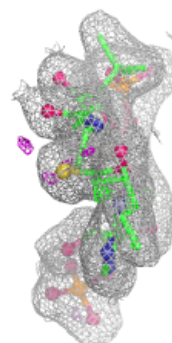
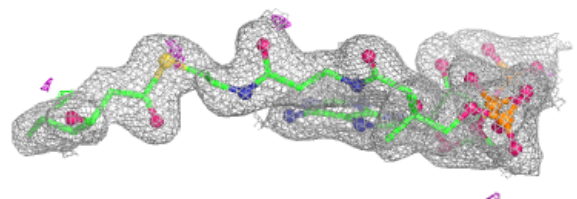
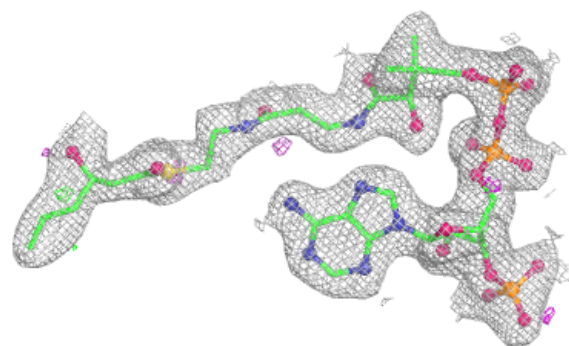


Electron density around 3H9 C 301:

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

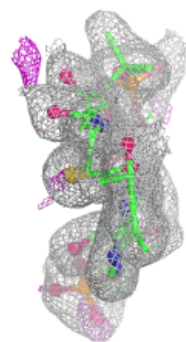
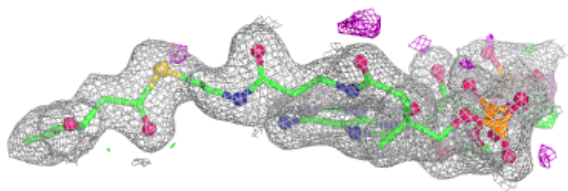
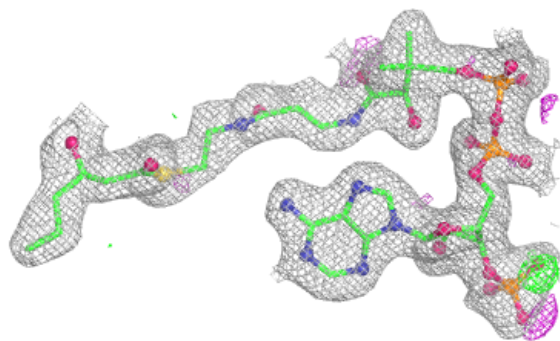
**Electron density around 3H9 E 301:**

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



Electron density around 3H9 A 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.