



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 04:21 pm BST

PDB ID : 9RGT / pdb_00009rgt
Title : Crystal Structure of Rattus norvegicus Enoyl-CoA Hydratase in complex with 3S-hydroxydecanoyl-CoA
Authors : Dalwani, S.; Wierenga, R.K.
Deposited on : 2025-06-07
Resolution : 2.00 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

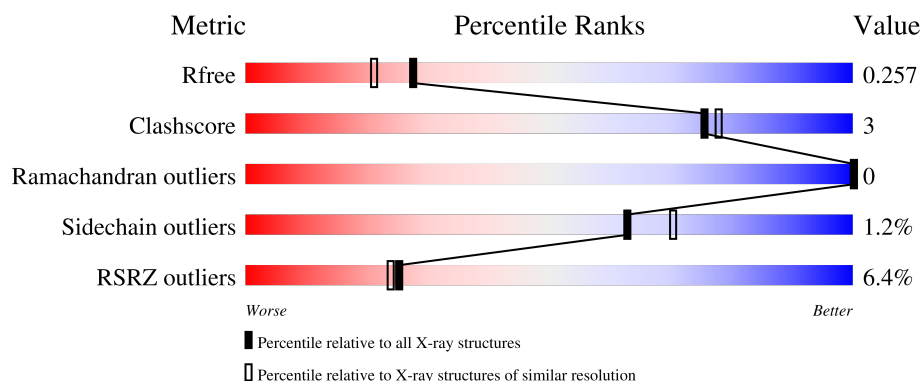
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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>6%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	290	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>5%</div> <div>12%</div> </div> </div>
1	C	290	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>5%</div> <div>12%</div> </div> </div>
1	D	290	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	E	290	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	290	<div><div></div><div>4%</div><div>81%</div><div>7%</div><div>12%</div></div>

2 Entry composition [i](#)

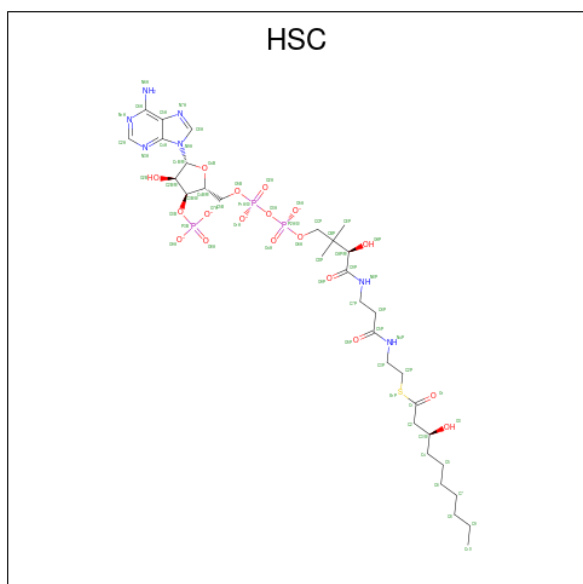
There are 3 unique types of molecules in this entry. The entry contains 12549 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	255	Total	C	N	O	S	0	0	0
			1937	1219	333	372	13			
1	B	255	Total	C	N	O	S	0	0	0
			1938	1219	333	373	13			
1	C	254	Total	C	N	O	S	0	0	0
			1927	1213	330	371	13			
1	D	260	Total	C	N	O	S	0	1	0
			1981	1248	340	379	14			
1	E	258	Total	C	N	O	S	0	0	0
			1965	1239	337	376	13			
1	F	254	Total	C	N	O	S	0	0	0
			1927	1213	330	371	13			

- Molecule 2 is (S)-3-HYDROXYDECANOYL-COA (CCD ID: HSC) (formula: $C_{31}H_{50}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 60	C 31	N 7	O 18	P 3	S 1	0	0
2	B	1	Total 60	C 31	N 7	O 18	P 3	S 1	0	0
2	C	1	Total 60	C 31	N 7	O 18	P 3	S 1	0	0
2	E	1	Total 60	C 31	N 7	O 18	P 3	S 1	0	0
2	F	1	Total 60	C 31	N 7	O 18	P 3	S 1	0	0

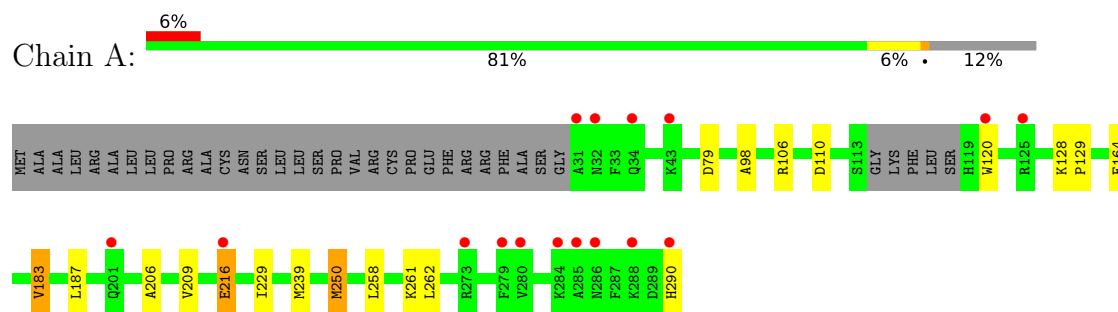
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total 100	O 100	0	0
3	B	109	Total 109	O 109	0	0
3	C	74	Total 74	O 74	0	0
3	D	86	Total 86	O 86	0	0
3	E	102	Total 102	O 102	0	0
3	F	103	Total 103	O 103	0	0

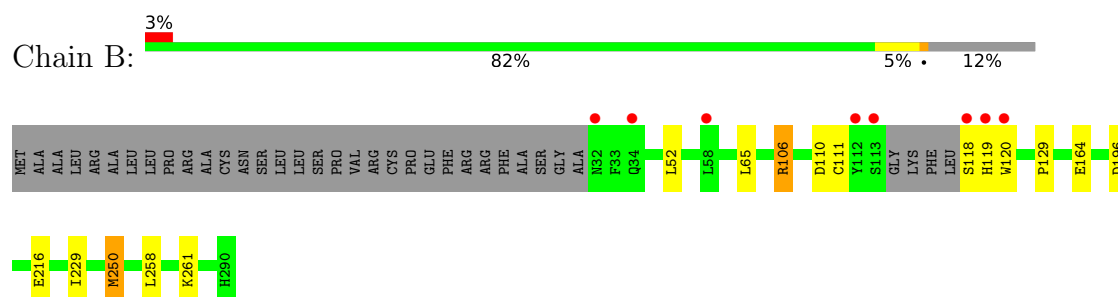
3 Residue-property plots [i](#)

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.

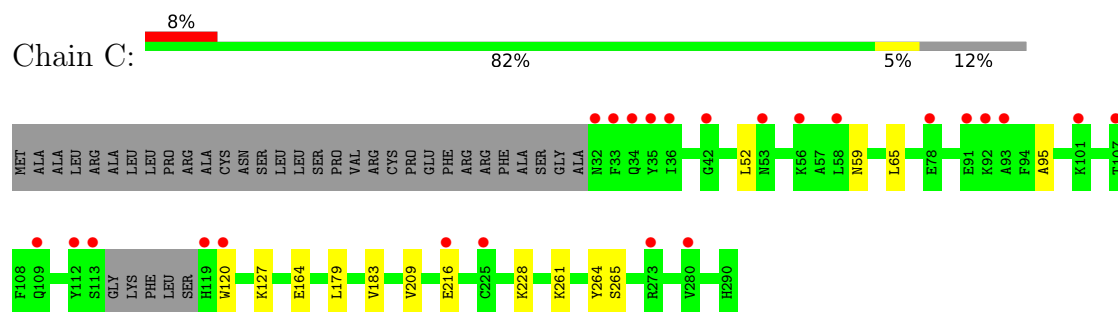
- Molecule 1: Enoyl-CoA hydratase, mitochondrial



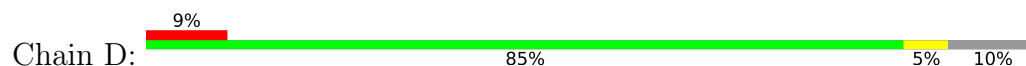
- Molecule 1: Enoyl-CoA hydratase, mitochondrial

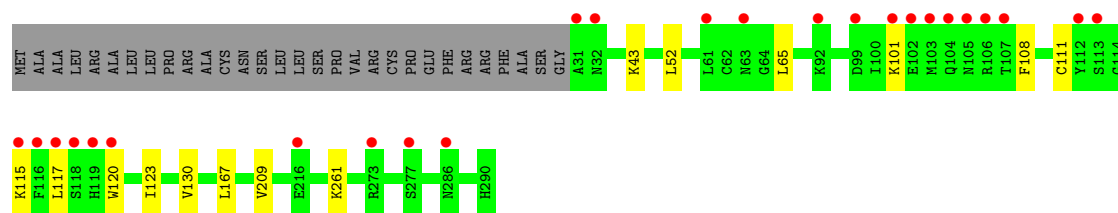


- Molecule 1: Enoyl-CoA hydratase, mitochondrial

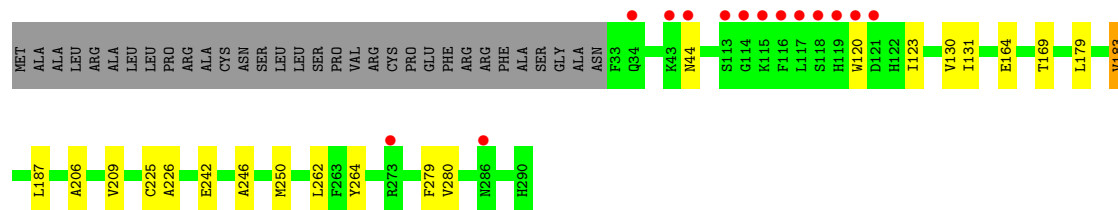
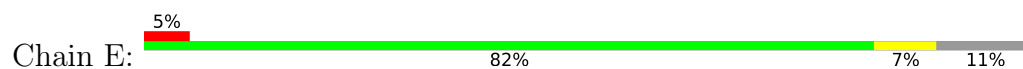


- Molecule 1: Enoyl-CoA hydratase, mitochondrial

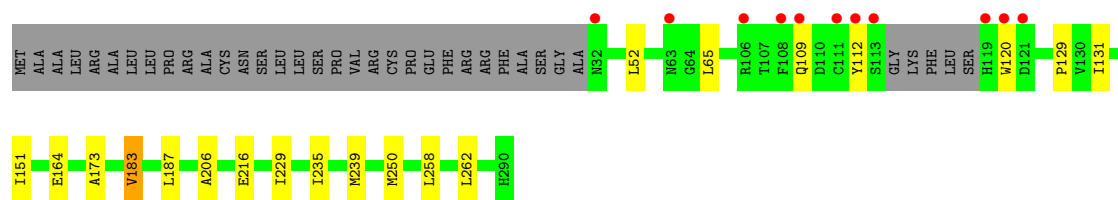
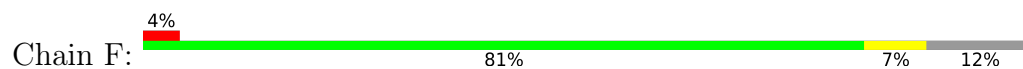




- Molecule 1: Enoyl-CoA hydratase, mitochondrial



- Molecule 1: Enoyl-CoA hydratase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.79Å 94.48Å 248.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.38 – 2.00 73.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (73.38-2.00) 95.9 (73.38-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.258 0.230 , 0.257	Depositor DCC
R_{free} test set	6071 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12549	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HSC

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	0.11	0/1962	0.30	0/2635
1	B	0.11	0/1963	0.30	0/2636
1	C	0.10	0/1951	0.29	0/2620
1	D	0.11	0/2011	0.30	0/2701
1	E	0.16	0/1992	0.33	0/2675
1	F	0.12	0/1951	0.31	0/2620
All	All	0.12	0/11830	0.30	0/15887

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1937	0	1956	16	0
1	B	1938	0	1956	13	0
1	C	1927	0	1946	11	0
1	D	1981	0	2007	10	0
1	E	1965	0	1991	17	0
1	F	1927	0	1946	15	0
2	A	60	0	50	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	60	0	50	3	0
2	C	60	0	50	3	0
2	E	60	0	50	4	0
2	F	60	0	50	5	0
3	A	100	0	0	1	0
3	B	109	0	0	1	0
3	C	74	0	0	0	0
3	D	86	0	0	0	0
3	E	102	0	0	2	0
3	F	103	0	0	0	0
All	All	12549	0	12052	71	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 3.

All (71) 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:B:106:ARG:NH1	1:B:110:ASP:OD2	2.21	0.74
1:A:250:MET:HE1	1:A:258:LEU:HD22	1.72	0.70
1:A:106:ARG:NH1	1:A:110:ASP:OD2	2.24	0.70
1:F:250:MET:HE1	1:F:258:LEU:HD22	1.75	0.67
1:C:52:LEU:HD22	1:C:65:LEU:HD21	1.81	0.61
1:B:250:MET:HE1	1:B:258:LEU:HD22	1.83	0.60
1:F:52:LEU:HD22	1:F:65:LEU:HD21	1.83	0.60
1:A:120:TRP:CD2	2:A:301:HSC:H6	2.37	0.60
1:A:216:GLU:H	1:A:216:GLU:CD	2.09	0.60
1:A:183:VAL:HG22	1:A:206:ALA:HB1	1.83	0.60
1:E:246:ALA:HB1	1:E:250:MET:HE3	1.83	0.60
1:F:183:VAL:HG13	1:F:187:LEU:HB3	1.84	0.58
1:F:120:TRP:HB3	2:F:301:HSC:H8	1.86	0.58
1:A:129:PRO:HG2	1:A:229:ILE:HG21	1.85	0.58
1:B:129:PRO:HG2	1:B:229:ILE:HG21	1.86	0.57
1:C:120:TRP:CD1	2:C:301:HSC:H8A	2.39	0.57
1:E:183:VAL:HG13	1:E:187:LEU:HB3	1.86	0.56
1:B:52:LEU:HD22	1:B:65:LEU:HD21	1.89	0.55
1:E:120:TRP:CE3	2:E:301:HSC:H6	2.42	0.54
1:A:164:GLU:OE2	2:A:301:HSC:O3	2.26	0.53
1:E:120:TRP:CH2	2:E:301:HSC:H5A	2.44	0.52
1:E:183:VAL:HG22	1:E:206:ALA:HB1	1.92	0.52
1:E:44:ASN:ND2	3:E:404:HOH:O	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ILE:HD11	1:E:130:VAL:HG11	1.92	0.51
1:B:261:LYS:HD3	1:F:262:LEU:HD21	1.93	0.51
1:D:167:LEU:HD22	1:E:279:PHE:HB2	1.92	0.51
1:D:52:LEU:HD22	1:D:65:LEU:HD21	1.93	0.50
1:E:225:CYS:HB2	3:E:487:HOH:O	2.11	0.50
1:C:261:LYS:HD3	1:E:262:LEU:HD21	1.93	0.50
1:D:117:LEU:HD22	1:D:120:TRP:CE2	2.47	0.49
1:A:290:HIS:HB2	1:F:109:GLN:HG2	1.95	0.48
1:E:164:GLU:HB3	1:E:169:THR:HG23	1.96	0.48
1:C:120:TRP:CH2	2:C:301:HSC:H5A	2.49	0.48
1:E:120:TRP:CG	2:E:301:HSC:H8	2.49	0.48
1:B:164:GLU:OE2	2:B:301:HSC:O3	2.31	0.47
1:B:120:TRP:CZ3	2:B:301:HSC:H5A	2.49	0.47
1:B:118:SER:OG	1:B:119:HIS:N	2.47	0.47
1:C:265:SER:HB3	1:D:108:PHE:CZ	2.50	0.47
1:D:123:ILE:HD11	1:D:130:VAL:HG11	1.98	0.46
1:B:120:TRP:HB3	2:B:301:HSC:H8A	1.98	0.46
1:A:261:LYS:NZ	3:A:404:HOH:O	2.40	0.46
1:A:120:TRP:CH2	2:A:301:HSC:H5A	2.50	0.46
1:A:183:VAL:HG13	1:A:187:LEU:HB3	1.97	0.46
1:C:127:LYS:HD2	1:D:115:LYS:HE2	1.98	0.46
1:C:164:GLU:OE2	2:C:301:HSC:O3	2.33	0.45
1:A:120:TRP:CD1	2:A:301:HSC:H8A	2.52	0.45
1:A:262:LEU:HD21	1:D:261:LYS:HD3	1.98	0.45
1:B:106:ARG:NH1	1:B:106:ARG:HA	2.31	0.45
1:E:164:GLU:OE2	2:E:301:HSC:O3	2.27	0.45
1:F:173:ALA:HB2	2:F:301:HSC:H6	1.99	0.45
1:A:98:ALA:HB2	2:A:301:HSC:H5	1.99	0.44
1:A:79:ASP:O	1:A:128:LYS:NZ	2.50	0.44
1:F:120:TRP:CG	2:F:301:HSC:H8	2.52	0.44
1:F:129:PRO:HG2	1:F:229:ILE:HG21	1.99	0.44
1:A:239:MET:HE2	1:F:112:TYR:CE2	2.53	0.44
1:E:131:ILE:HD12	1:E:226:ALA:HB2	2.00	0.43
1:F:131:ILE:HG12	1:F:151:ILE:HB	2.00	0.43
1:F:164:GLU:OE2	2:F:301:HSC:O3	2.35	0.43
1:F:183:VAL:HG22	1:F:206:ALA:HB1	2.00	0.43
1:B:196:ASP:O	3:B:401:HOH:O	2.22	0.42
1:F:235:ILE:HG12	1:F:239:MET:HE3	2.02	0.42
1:D:101:LYS:HE3	1:E:280:VAL:HG13	2.02	0.42
1:B:216:GLU:OE1	1:B:216:GLU:N	2.50	0.42
1:D:43:LYS:HE2	1:D:43:LYS:HB3	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:CYS:HB3	1:E:264:TYR:CD1	2.54	0.41
1:C:59:ASN:HB2	1:C:95:ALA:HA	2.01	0.41
1:C:216:GLU:H	1:C:216:GLU:CD	2.28	0.41
1:C:179:LEU:O	1:C:183:VAL:HG22	2.20	0.41
1:F:120:TRP:CD2	2:F:301:HSC:H7A	2.55	0.41
1:B:111:CYS:HB3	1:C:264:TYR:CD1	2.57	0.40
1:E:179:LEU:O	1:E:183:VAL:HB	2.21	0.40

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	251/290 (87%)	247 (98%)	4 (2%)	0	100	100
1	B	251/290 (87%)	245 (98%)	6 (2%)	0	100	100
1	C	250/290 (86%)	245 (98%)	5 (2%)	0	100	100
1	D	259/290 (89%)	254 (98%)	5 (2%)	0	100	100
1	E	256/290 (88%)	251 (98%)	5 (2%)	0	100	100
1	F	250/290 (86%)	245 (98%)	5 (2%)	0	100	100
All	All	1517/1740 (87%)	1487 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/229 (87%)	196 (98%)	4 (2%)	48	54
1	B	201/229 (88%)	199 (99%)	2 (1%)	68	75
1	C	199/229 (87%)	197 (99%)	2 (1%)	68	75
1	D	206/229 (90%)	205 (100%)	1 (0%)	81	87
1	E	204/229 (89%)	201 (98%)	3 (2%)	57	64
1	F	199/229 (87%)	197 (99%)	2 (1%)	68	75
All	All	1209/1374 (88%)	1195 (99%)	14 (1%)	63	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	VAL
1	A	209	VAL
1	A	216	GLU
1	A	250	MET
1	B	106	ARG
1	B	250	MET
1	C	209	VAL
1	C	228	LYS
1	D	209	VAL
1	E	183	VAL
1	E	209	VAL
1	E	242	GLU
1	F	183	VAL
1	F	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	159	GLN
1	B	104	GLN
1	B	159	GLN
1	C	104	GLN
1	C	159	GLN
1	D	105	ASN
1	D	162	GLN
1	E	205	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	104	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](#)

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	$\# Z > 2$
2	HSC	E	301	-	56,62,62	0.43	0	78,89,89	0.83	2 (2%)
2	HSC	F	301	-	56,62,62	0.44	0	78,89,89	0.81	1 (1%)
2	HSC	B	301	-	56,62,62	0.43	0	78,89,89	0.81	1 (1%)
2	HSC	A	301	-	56,62,62	0.42	0	78,89,89	0.81	1 (1%)
2	HSC	C	301	-	56,62,62	0.44	0	78,89,89	0.81	1 (1%)

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	HSC	E	301	-	-	4/62/78/78	0/3/3/3
2	HSC	F	301	-	-	3/62/78/78	0/3/3/3
2	HSC	B	301	-	-	3/62/78/78	0/3/3/3
2	HSC	A	301	-	-	7/62/78/78	0/3/3/3
2	HSC	C	301	-	-	5/62/78/78	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	HSC	O1A-P1A-O2A	-3.40	95.43	112.24
2	B	301	HSC	O1A-P1A-O2A	-3.32	95.81	112.24
2	C	301	HSC	O1A-P1A-O2A	-3.28	96.00	112.24
2	A	301	HSC	O1A-P1A-O2A	-3.28	96.02	112.24
2	E	301	HSC	O1A-P1A-O2A	-3.23	96.26	112.24
2	E	301	HSC	O2B-C2B-C3B	2.09	117.11	111.17

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	HSC	C6-C7-C8-C9
2	E	301	HSC	C4-C5-C6-C7
2	A	301	HSC	C5-C6-C7-C8
2	A	301	HSC	C4-C5-C6-C7
2	B	301	HSC	O3-C3-C4-C5
2	C	301	HSC	C4-C5-C6-C7
2	C	301	HSC	C5-C6-C7-C8
2	C	301	HSC	C7-C8-C9-C10
2	A	301	HSC	C5B-O5B-P1A-O3A
2	E	301	HSC	C1-C2-C3-C4
2	B	301	HSC	C4-C5-C6-C7
2	A	301	HSC	C6-C7-C8-C9
2	B	301	HSC	C2-C3-C4-C5
2	A	301	HSC	C3-C4-C5-C6
2	F	301	HSC	C5-C6-C7-C8
2	C	301	HSC	O3-C3-C4-C5
2	F	301	HSC	O3-C3-C4-C5
2	A	301	HSC	C7-C8-C9-C10
2	E	301	HSC	C1-C2-C3-O3
2	E	301	HSC	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	301	HSC	C1-C2-C3-C4
2	C	301	HSC	C1-C2-C3-C4

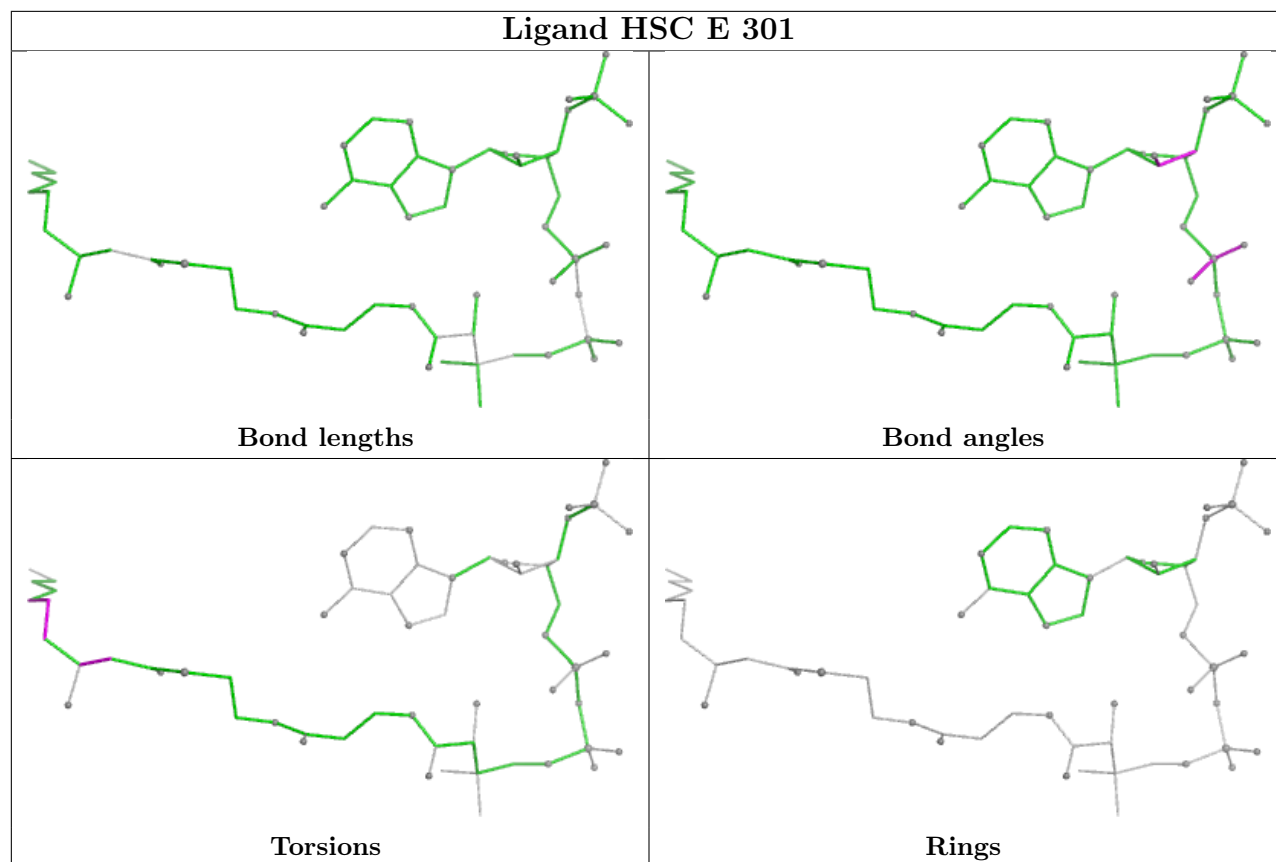
There are no ring outliers.

5 monomers are involved in 20 short contacts:

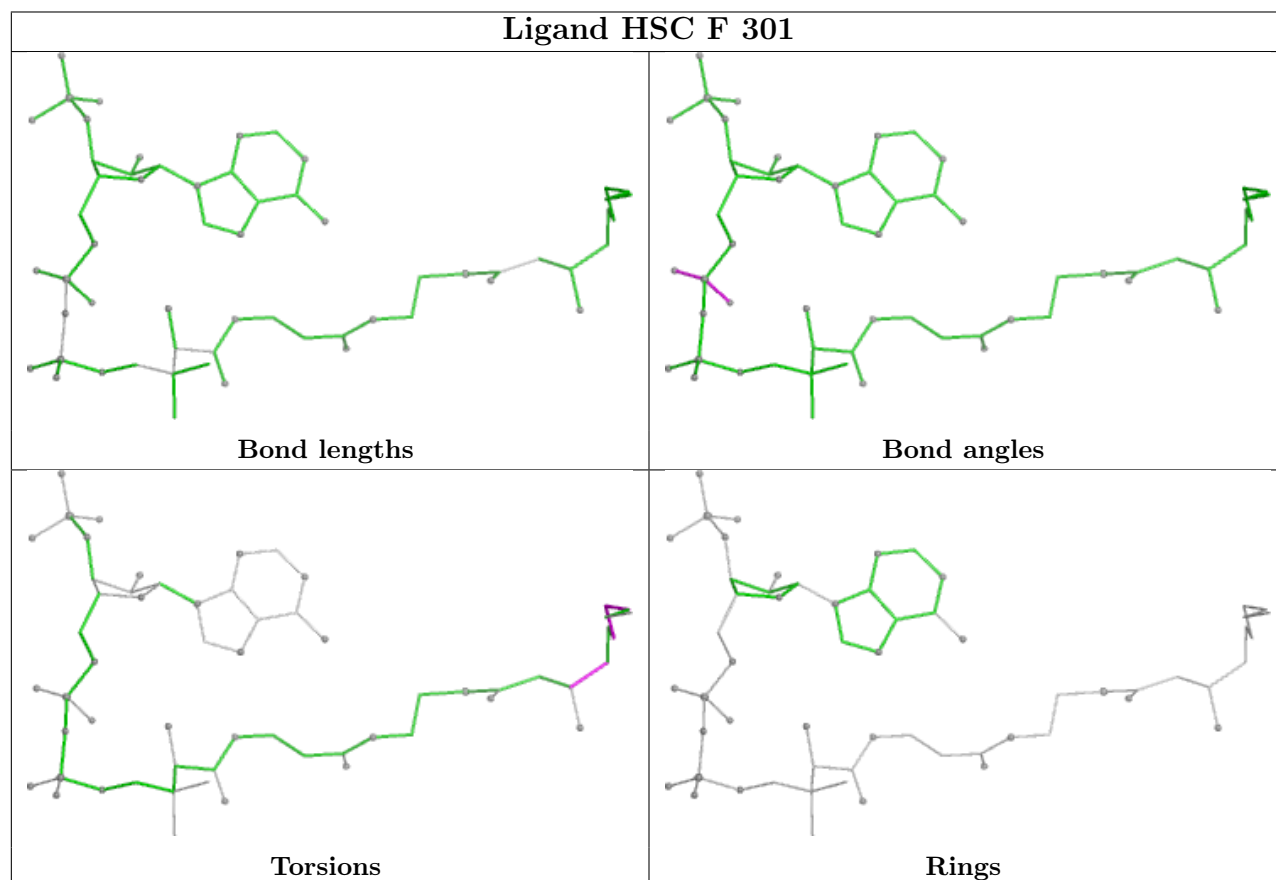
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	HSC	4	0
2	F	301	HSC	5	0
2	B	301	HSC	3	0
2	A	301	HSC	5	0
2	C	301	HSC	3	0

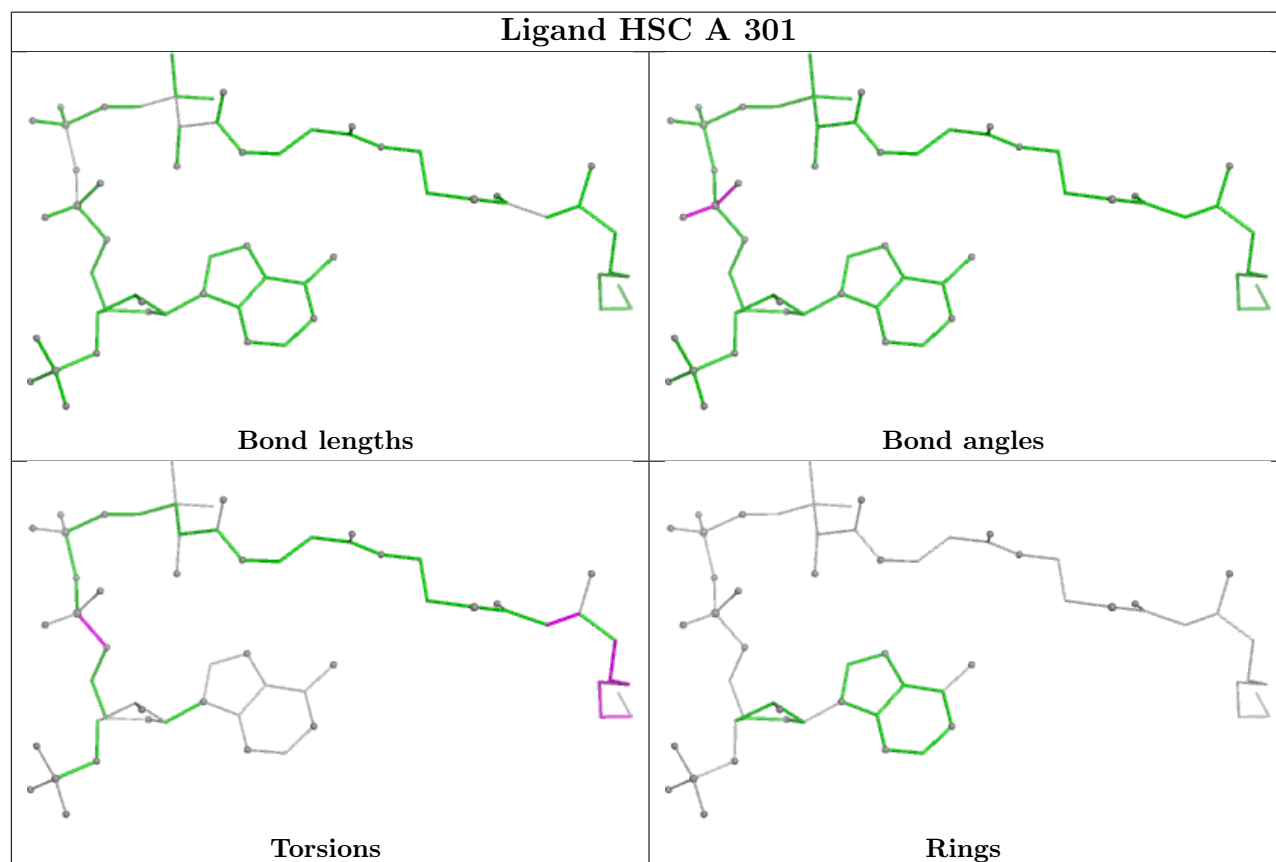
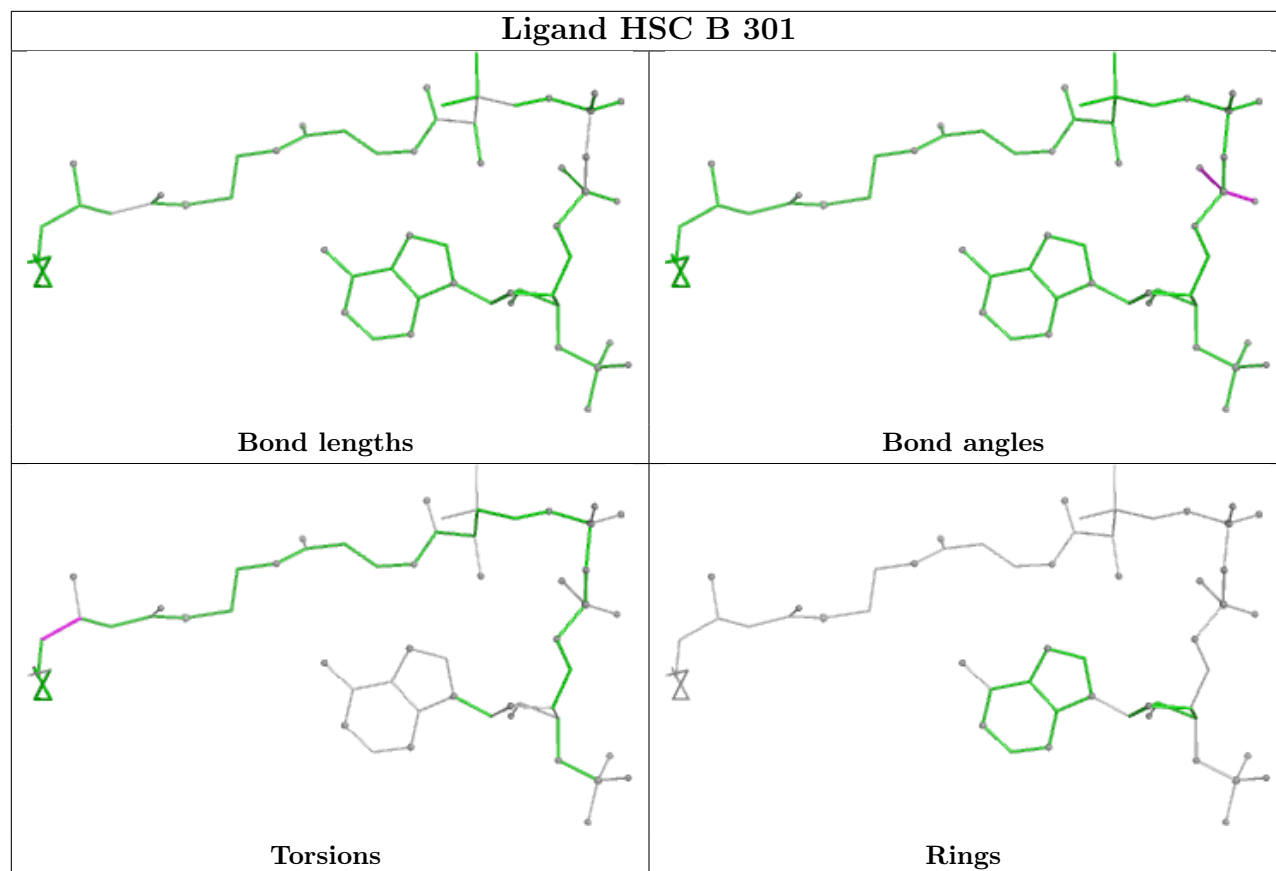
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

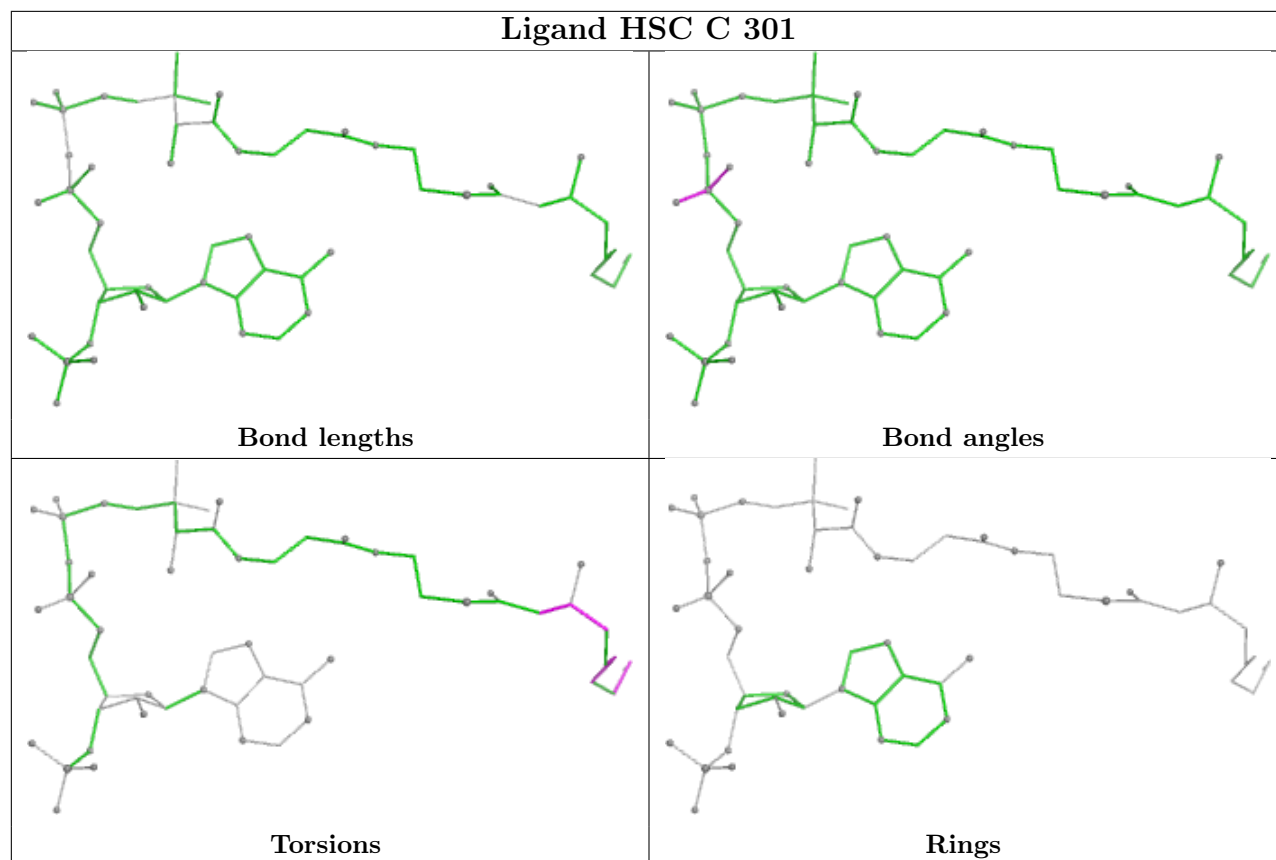
Ligand HSC E 301



Ligand HSC F 301







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

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	255/290 (87%)	0.52	16 (6%) 26 24	6, 18, 36, 53	0
1	B	255/290 (87%)	0.30	8 (3%) 51 50	7, 15, 32, 46	0
1	C	254/290 (87%)	0.78	24 (9%) 14 13	8, 23, 40, 55	0
1	D	260/290 (89%)	0.61	25 (9%) 13 12	9, 18, 44, 63	1 (0%)
1	E	258/290 (88%)	0.34	14 (5%) 31 30	6, 15, 32, 66	0
1	F	254/290 (87%)	0.32	11 (4%) 40 39	6, 13, 36, 47	0
All	All	1536/1740 (88%)	0.48	98 (6%) 25 24	6, 17, 38, 66	1 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	112	TYR	5.5
1	D	117	LEU	5.3
1	F	120	TRP	5.2
1	D	120	TRP	5.0
1	A	43	LYS	5.0
1	E	117	LEU	5.0
1	A	31	ALA	4.8
1	F	32	ASN	4.7
1	C	120	TRP	4.6
1	D	31	ALA	4.5
1	E	114	GLY	4.4
1	D	105	ASN	4.2
1	B	32	ASN	4.2
1	C	112	TYR	4.2
1	C	113	SER	4.1
1	C	119	HIS	4.0
1	E	43	LYS	4.0
1	E	115	LYS	4.0
1	D	112	TYR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	119	HIS	3.7
1	F	113	SER	3.6
1	B	118	SER	3.6
1	D	103	MET	3.5
1	B	120	TRP	3.5
1	C	34	GLN	3.4
1	D	99	ASP	3.4
1	E	113	SER	3.4
1	A	284	LYS	3.3
1	D	286	ASN	3.3
1	E	116	PHE	3.3
1	C	35	TYR	3.2
1	C	32	ASN	3.2
1	B	112	TYR	3.2
1	D	113	SER	3.1
1	F	106	ARG	3.1
1	D	118	SER	3.1
1	A	120	TRP	3.0
1	D	101	LYS	3.0
1	C	273	ARG	3.0
1	C	33	PHE	3.0
1	A	280	VAL	2.9
1	E	118	SER	2.9
1	A	290	HIS	2.9
1	D	116	PHE	2.9
1	D	61	LEU	2.8
1	F	109	GLN	2.8
1	F	111	CYS	2.8
1	A	286	ASN	2.7
1	C	109	GLN	2.7
1	D	104	GLN	2.7
1	D	92	LYS	2.7
1	B	119	HIS	2.7
1	F	119	HIS	2.7
1	D	216	GLU	2.6
1	A	201	GLN	2.6
1	D	63	ASN	2.6
1	D	107	THR	2.6
1	D	106	ARG	2.6
1	A	216	GLU	2.6
1	E	121	ASP	2.6
1	C	42	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	34	GLN	2.5
1	C	225	CYS	2.5
1	A	125	ARG	2.5
1	A	273	ARG	2.5
1	D	273	ARG	2.5
1	A	32	ASN	2.5
1	D	115	LYS	2.5
1	C	92	LYS	2.5
1	D	32	ASN	2.5
1	E	286	ASN	2.5
1	C	36	ILE	2.4
1	C	216	GLU	2.4
1	E	273	ARG	2.4
1	D	119	HIS	2.4
1	A	279	PHE	2.4
1	F	108	PHE	2.3
1	B	113	SER	2.2
1	A	288	LYS	2.2
1	C	56	LYS	2.2
1	A	285	ALA	2.2
1	D	102	GLU	2.2
1	C	280	VAL	2.2
1	C	91	GLU	2.2
1	E	34	GLN	2.2
1	B	58	LEU	2.2
1	C	93	ALA	2.1
1	A	34	GLN	2.1
1	C	58	LEU	2.1
1	D	277	SER	2.1
1	C	107	THR	2.1
1	E	120	TRP	2.1
1	C	78	GLU	2.1
1	C	53	ASN	2.1
1	F	121	ASP	2.0
1	E	44	ASN	2.0
1	F	63	ASN	2.0
1	C	101	LYS	2.0

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

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](#)

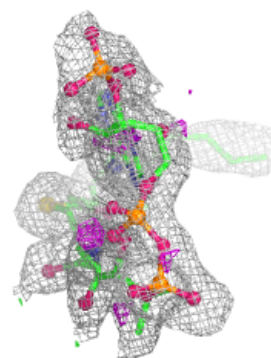
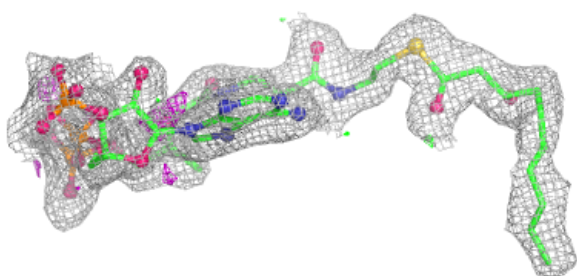
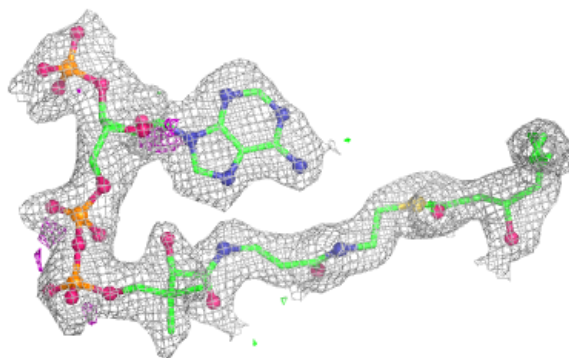
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HSC	B	301	60/60	0.87	0.12	15,28,46,52	0
2	HSC	F	301	60/60	0.87	0.12	16,27,45,50	0
2	HSC	C	301	60/60	0.88	0.12	18,30,44,47	0
2	HSC	E	301	60/60	0.94	0.08	6,13,22,29	0
2	HSC	A	301	60/60	0.94	0.09	6,14,26,30	0

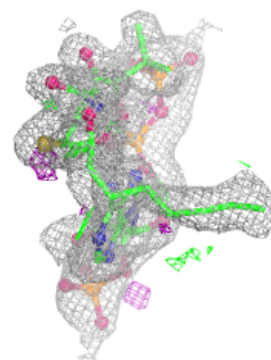
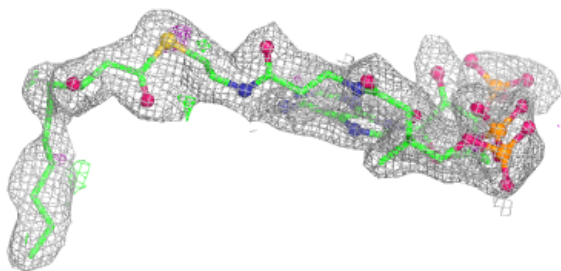
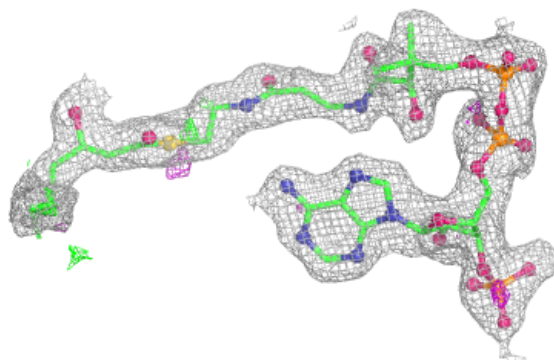
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HSC 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)

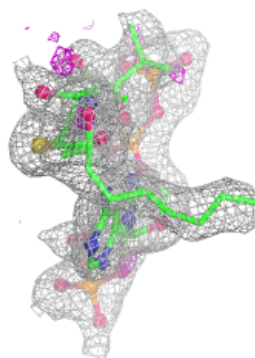
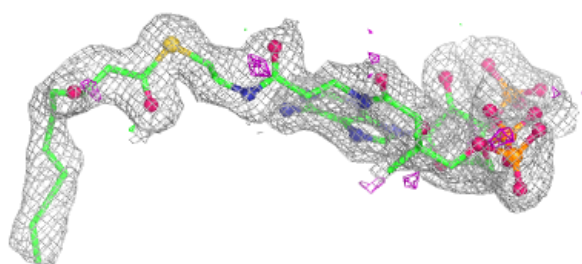
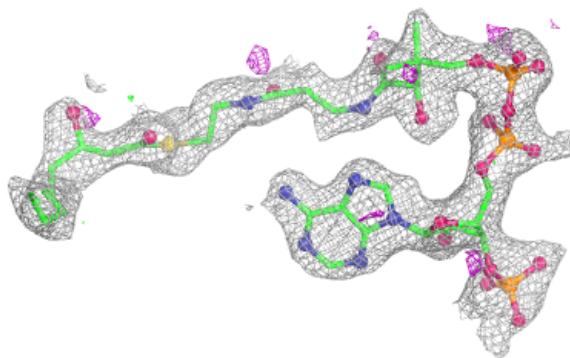
**Electron density around HSC F 301:**

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

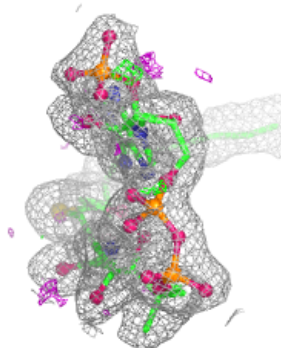
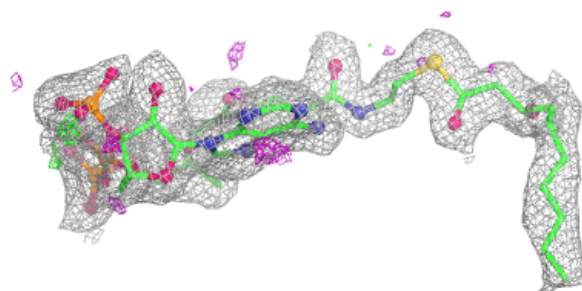
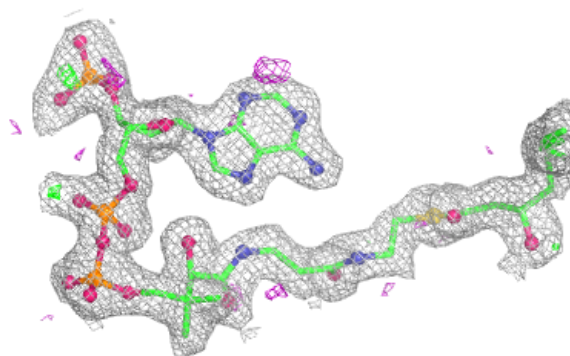


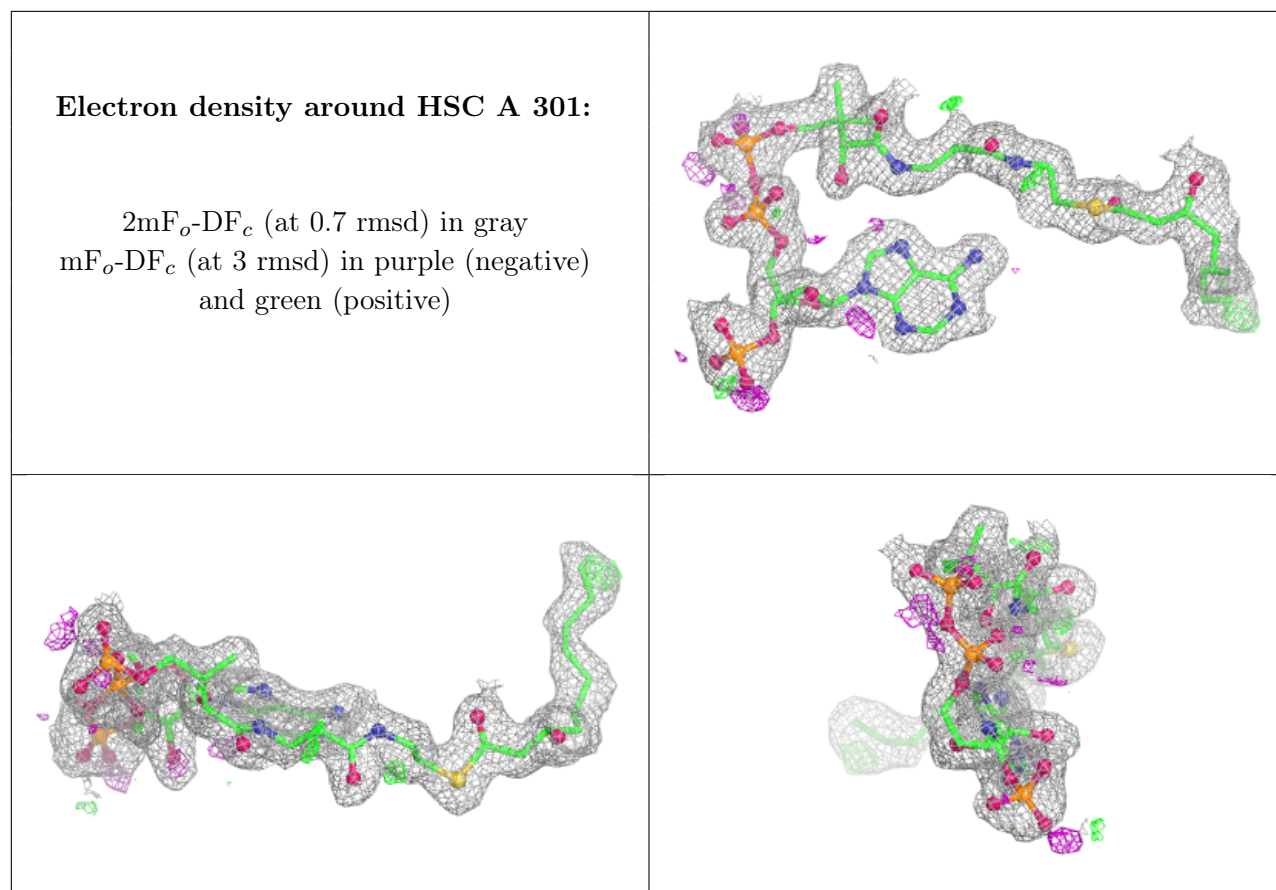
Electron density around HSC C 301:

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

**Electron density around HSC 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.