



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:03 AM UTC

PDB ID : 1UYS / pdb_00001uys
Title : Acetyl-CoA carboxylase carboxyltransferase domain in complex with inhibitor haloxyfop
Authors : Zhang, H.; Tweel, B.; Tong, L.
Deposited on : 2004-03-02
Resolution : 2.80 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 ⓘ](#)) 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

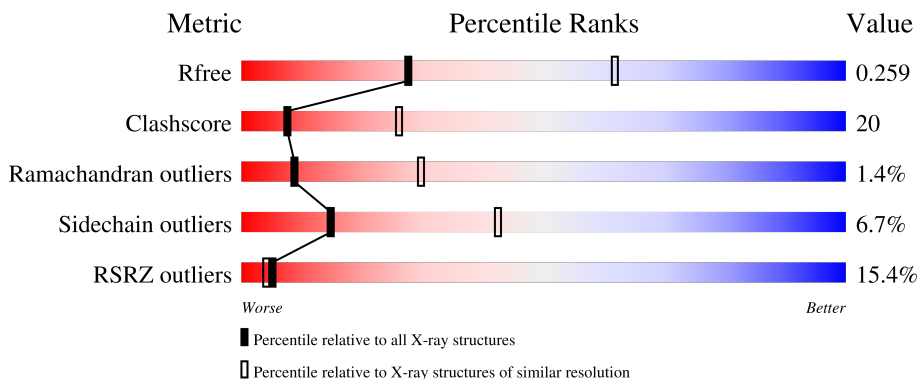
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	737	12% 56% 32% 9%
1	B	737	15% 53% 34% 9%
1	C	737	14% 52% 33% 10%

2 Entry composition [i](#)

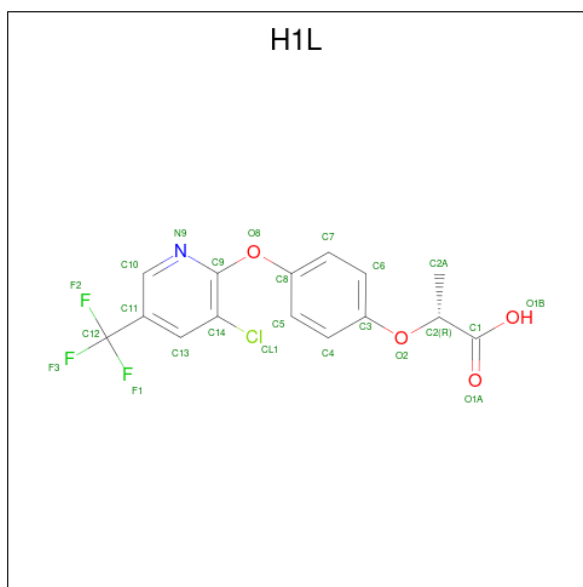
There are 3 unique types of molecules in this entry. The entry contains 16130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA CARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	B	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	C	660	Total	C	N	O	S	Se	0	0	1
			5248	3343	903	984	2	16			

- Molecule 2 is (2R)-2-(4-{[3-chloro-5-(trifluoromethyl)pyridin-2-yl]oxy}phenoxy)propanoic acid (CCD ID: H1L) (formula: C₁₅H₁₁ClF₃NO₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	C	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		

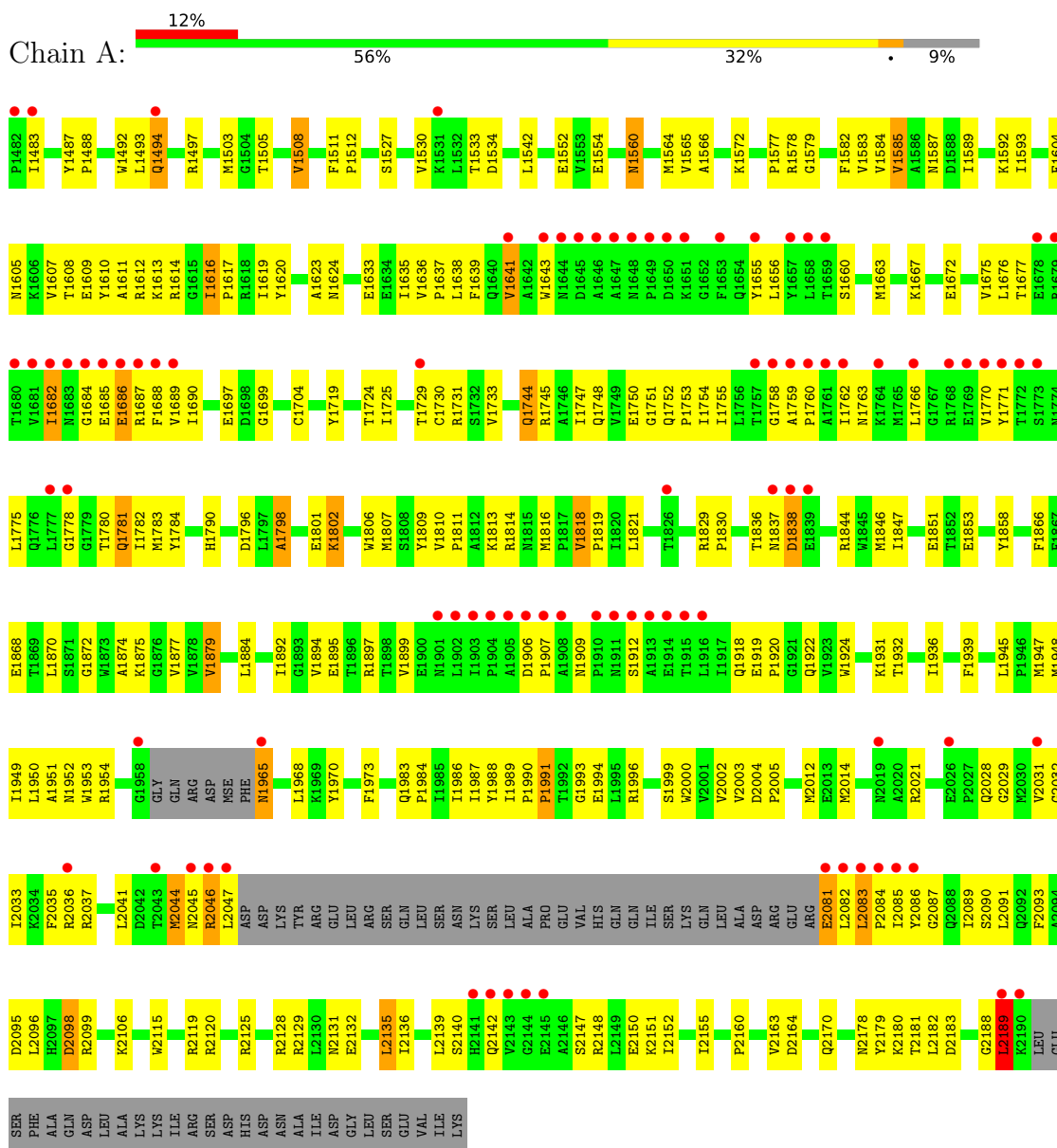
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	50	Total 50	O 50	0	0
3	C	39	Total 39	O 39	0	0

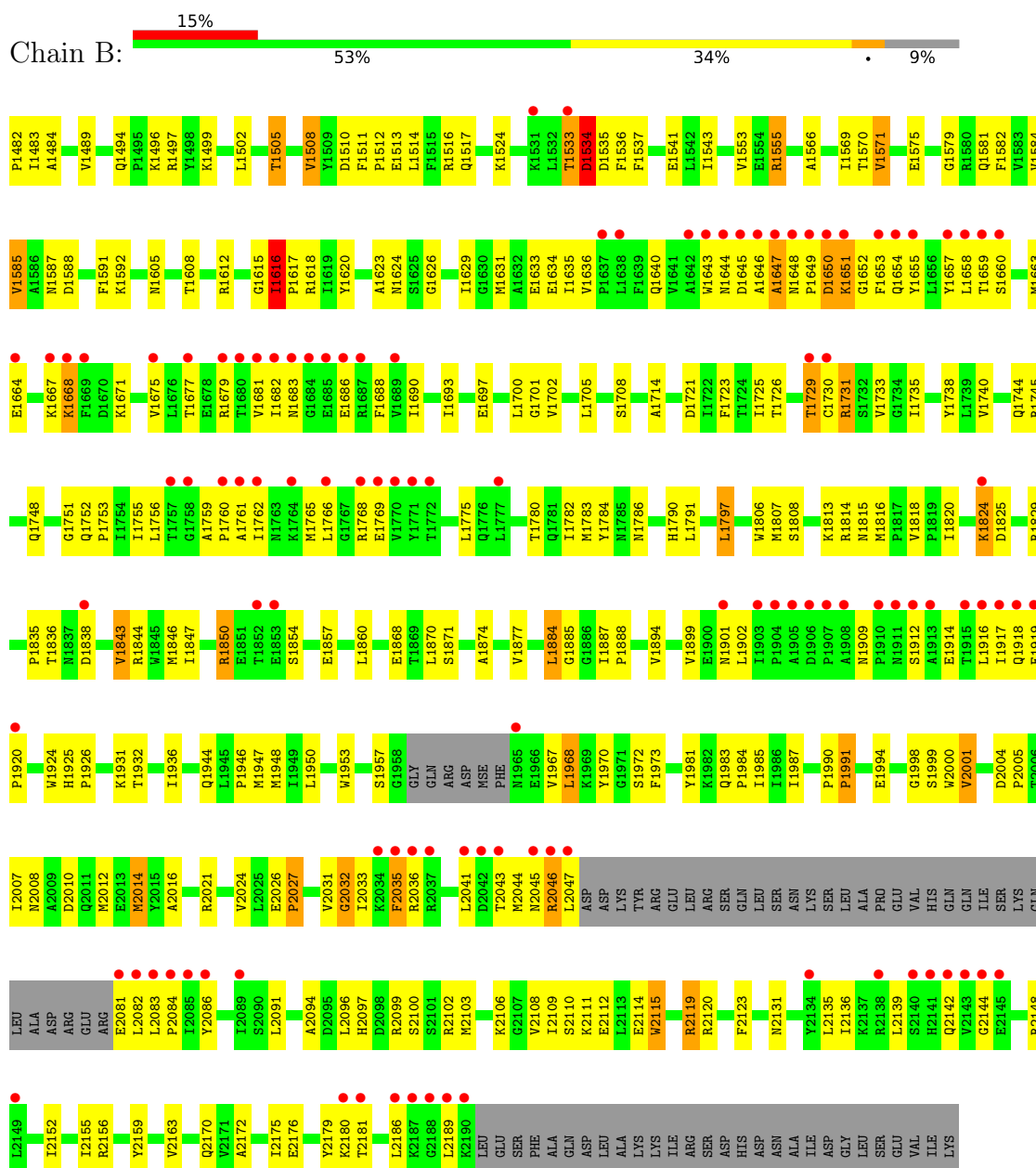
3 Residue-property plots

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.

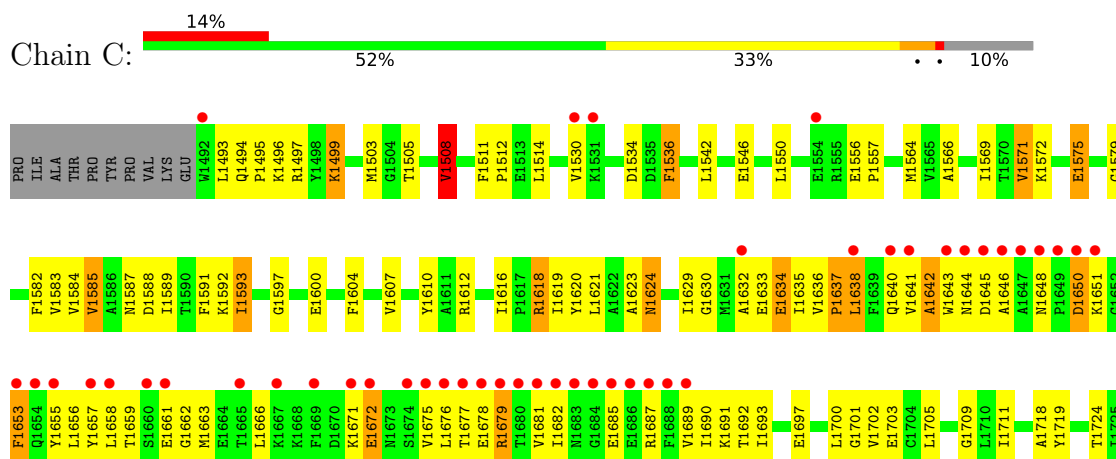
• Molecule 1: ACETYL-COA CARBOXYLASE



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SER	L2149	PRO	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148	
	L2152		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	R2156		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	P2160		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	V2163		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	D2164		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	D2168		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	E2169		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	Q2170		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
	W2174		ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148
L2182	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
K2185	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
L2186	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
L2189	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
K2190	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
LEU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
GLU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
SER	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
PHE	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ALA	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
GLN	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ASP	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
LEU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ASP	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
LEU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ASP	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
LEU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ASP	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
LEU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ASP	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
LEU	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W2115	R2128	E2132	E2133	I2136	G2144	Q2145	R2148		
ASP	ALA	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG	GLU	ARG	E2081	L2082	L2083	P2084	I2085	Y2086	G2087	Q2088	I2089	D2098	R2099	S2100	S2101	R2102	M2103	K2106	G2107	V2108	I2109	E2112	L2113	E2114	W211									

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.21Å 125.58Å 146.88Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	27.42 – 2.80 27.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.6 (27.42-2.80) 94.3 (27.42-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.252 0.225 , 0.259	Depositor DCC
R_{free} test set	10734 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16130	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: H1L

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	0.63	1/5429 (0.0%)	0.93	8/7332 (0.1%)
1	B	0.55	1/5429 (0.0%)	0.88	4/7332 (0.1%)
1	C	0.56	1/5347 (0.0%)	0.89	11/7218 (0.2%)
All	All	0.58	3/16205 (0.0%)	0.90	23/21882 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2189	LEU	C-N	-5.89	1.25	1.33
1	B	2189	LEU	C-N	-5.61	1.25	1.33
1	C	2189	LEU	C-N	-5.58	1.25	1.33

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1818	VAL	CA-C-N	9.07	131.18	119.84
1	A	1818	VAL	C-N-CA	9.07	131.18	119.84
1	A	1821	LEU	N-CA-C	7.79	120.18	107.32
1	C	1745	ARG	NE-CZ-NH2	7.53	125.98	119.20
1	C	1745	ARG	NE-CZ-NH1	-7.49	114.02	121.50

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	5326	0	5269	207	1
1	B	5326	0	5269	223	0
1	C	5248	0	5187	237	0
2	A	24	0	10	0	0
2	B	24	0	10	4	0
2	C	24	0	10	6	0
3	A	69	0	0	4	0
3	B	50	0	0	3	0
3	C	39	0	0	4	0
All	All	16130	0	15755	641	1

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 20.

The worst 5 of 641 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:C:1618:ARG:HG2	1:C:1618:ARG:HH11	1.25	1.01
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.40	1.00
1:C:1823:THR:HG22	1:C:1824:LYS:H	1.33	0.93
1:A:2045:ASN:HB2	1:A:2046:ARG:CZ	1.99	0.92
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.54	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:TYR:OH	1:A:1970:TYR:OH[2_555]	2.19	0.01

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	664/737 (90%)	602 (91%)	57 (9%)	5 (1%)	16	44
1	B	664/737 (90%)	597 (90%)	57 (9%)	10 (2%)	8	28
1	C	654/737 (89%)	576 (88%)	66 (10%)	12 (2%)	6	23
All	All	1982/2211 (90%)	1775 (90%)	180 (9%)	27 (1%)	9	30

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1991	PRO
1	B	1534	ASP
1	B	1650	ASP
1	B	1731	ARG
1	C	1632	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	567/611 (93%)	528 (93%)	39 (7%)	14	41
1	B	567/611 (93%)	527 (93%)	40 (7%)	13	39
1	C	558/611 (91%)	524 (94%)	34 (6%)	17	46
All	All	1692/1833 (92%)	1579 (93%)	113 (7%)	15	42

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1791	LEU
1	C	2081	GLU
1	B	2026	GLU
1	C	2046	ARG
1	C	1801	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1790	HIS
1	C	1922	GLN
1	C	2170	GLN
1	B	1599	GLN
1	B	1587	ASN

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](#)

3 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	H1L	C	3000	-	25,25,25	0.97	0	36,36,36	1.58	7 (19%)
2	H1L	A	3000	-	25,25,25	1.09	2 (8%)	36,36,36	1.49	8 (22%)
2	H1L	B	3000	-	25,25,25	1.31	4 (16%)	36,36,36	1.59	10 (27%)

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	H1L	C	3000	-	-	6/18/18/18	0/2/2/2
2	H1L	A	3000	-	-	4/18/18/18	0/2/2/2
2	H1L	B	3000	-	-	4/18/18/18	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	H1L	C7-C6	2.75	1.43	1.38
2	B	3000	H1L	C12-C11	2.39	1.54	1.49
2	B	3000	H1L	C5-C8	2.34	1.43	1.38
2	A	3000	H1L	O2-C3	-2.12	1.34	1.38
2	B	3000	H1L	C4-C3	2.03	1.42	1.38

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	H1L	C14-C9-N9	-4.31	118.93	122.69
2	A	3000	H1L	C11-C10-N9	-3.89	119.73	123.38
2	B	3000	H1L	C11-C10-N9	-3.43	120.16	123.38
2	C	3000	H1L	C11-C10-N9	-3.29	120.29	123.38
2	C	3000	H1L	O8-C9-N9	3.06	123.56	119.47

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3000	H1L	O1A-C1-C2-O2
2	A	3000	H1L	C1-C2-O2-C3
2	B	3000	H1L	C1-C2-O2-C3
2	C	3000	H1L	C1-C2-O2-C3
2	C	3000	H1L	C2A-C2-O2-C3

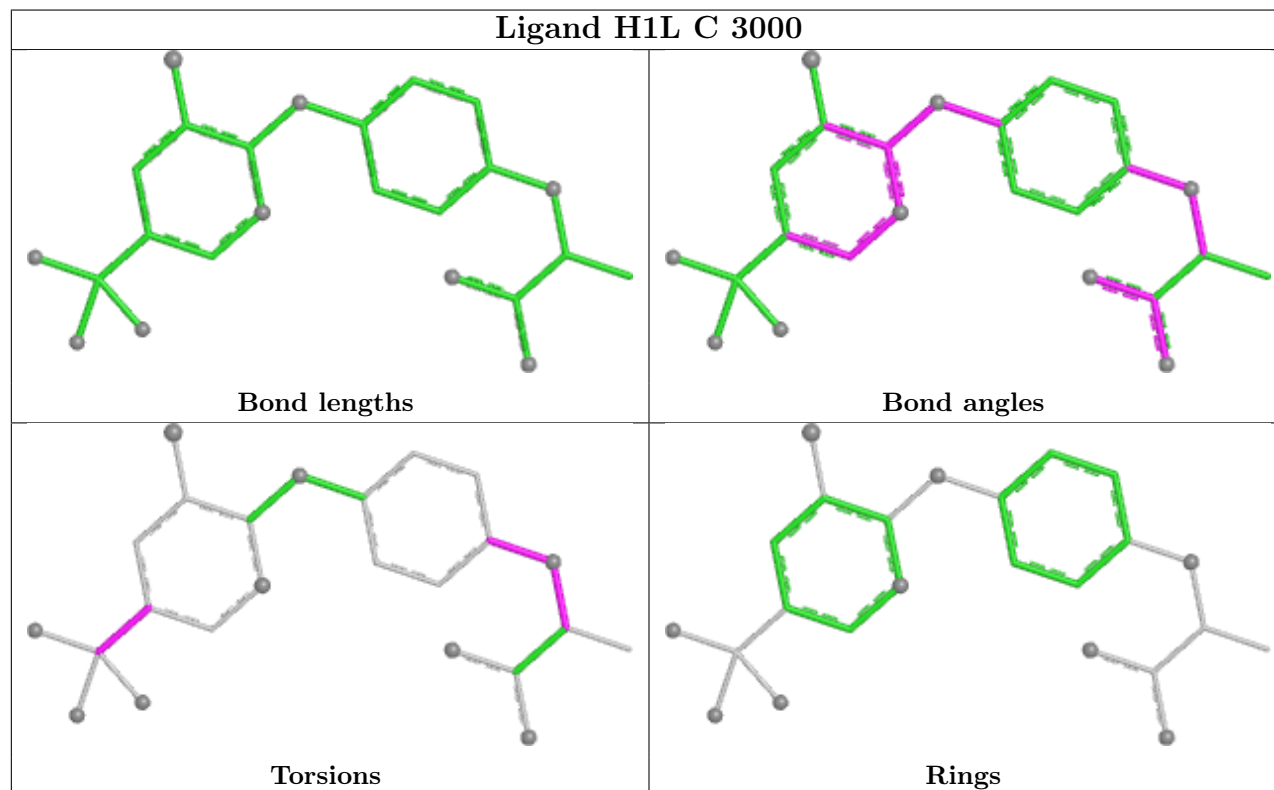
There are no ring outliers.

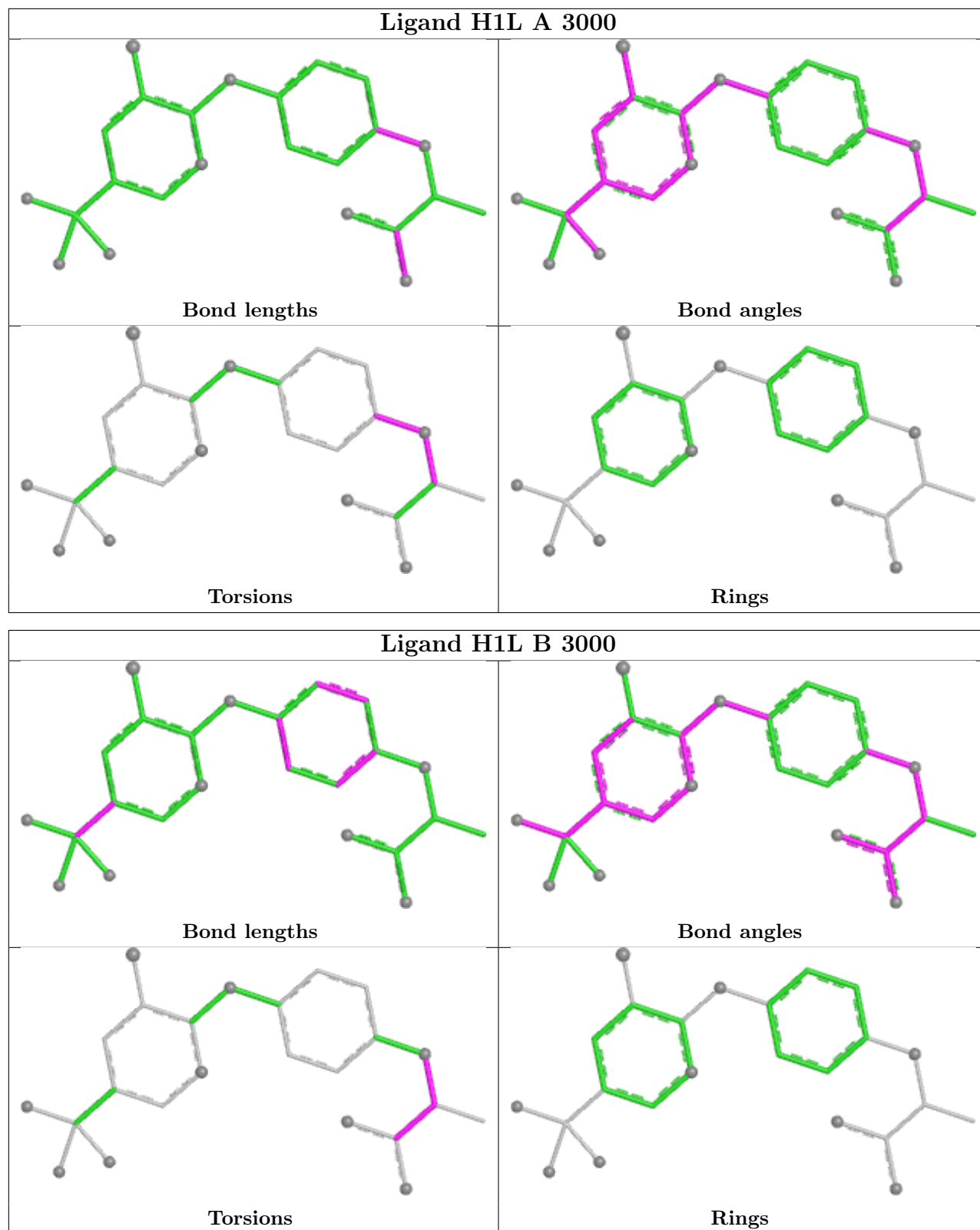
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	H1L	6	0
2	B	3000	H1L	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 ⓘ

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	654/737 (88%)	0.42	90 (13%) 6 5	13, 32, 98, 100	0
1	B	654/737 (88%)	0.57	107 (16%) 4 3	15, 37, 99, 100	0
1	C	644/737 (87%)	0.55	103 (15%) 5 4	14, 37, 100, 100	0
All	All	1952/2211 (88%)	0.52	300 (15%) 5 4	13, 36, 100, 100	0

The worst 5 of 300 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2047	LEU	8.7
1	C	2047	LEU	7.8
1	B	2047	LEU	7.8
1	C	1913	ALA	6.7
1	B	1908	ALA	6.6

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](#)

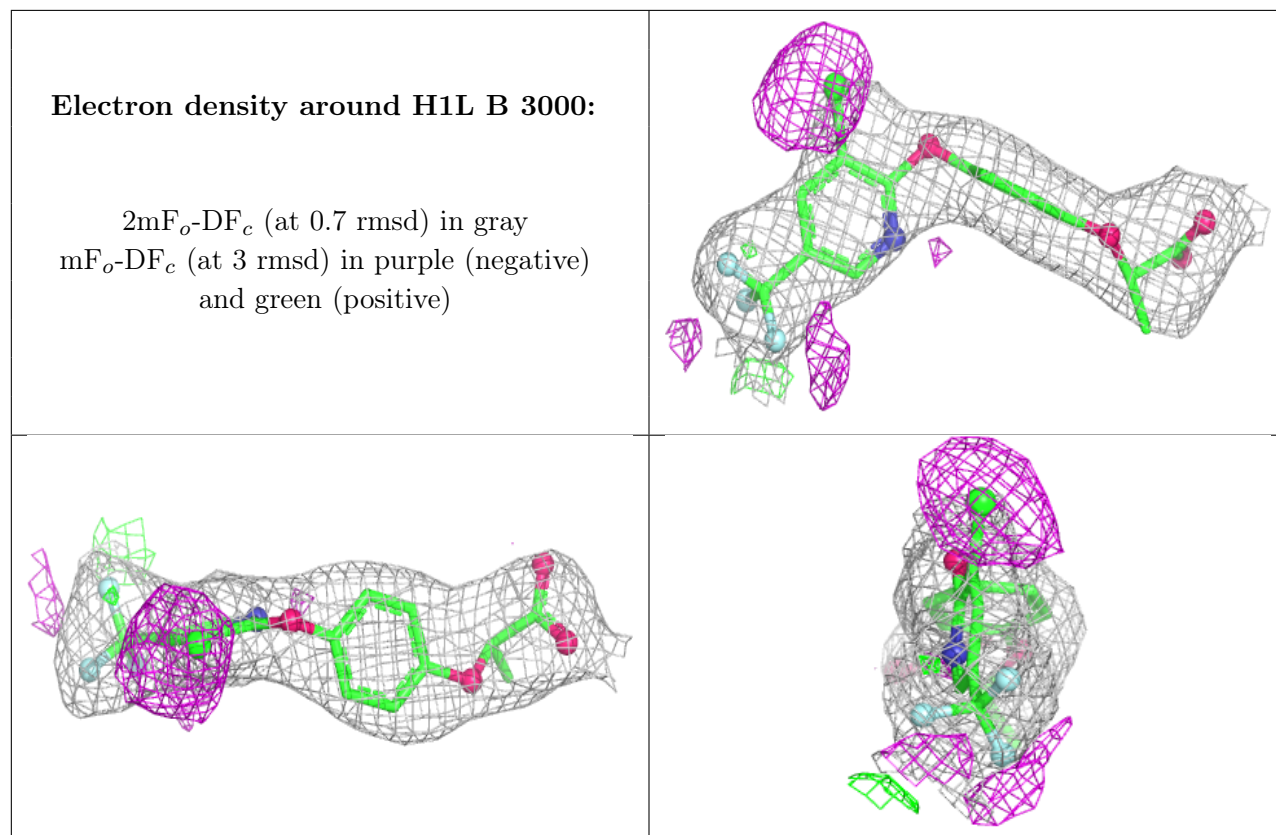
There are no oligosaccharides in this entry.

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.

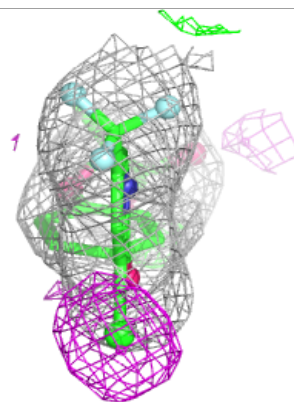
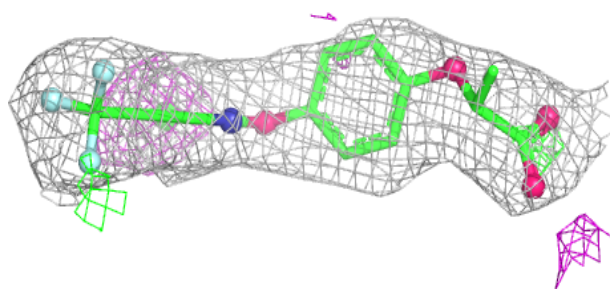
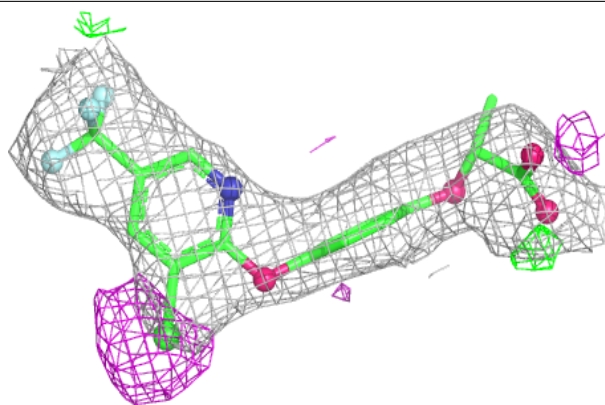
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	H1L	B	3000	24/24	0.86	0.17	44,49,59,71	0
2	H1L	C	3000	24/24	0.86	0.17	52,55,60,71	0
2	H1L	A	3000	24/24	0.90	0.13	29,38,45,54	0

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.

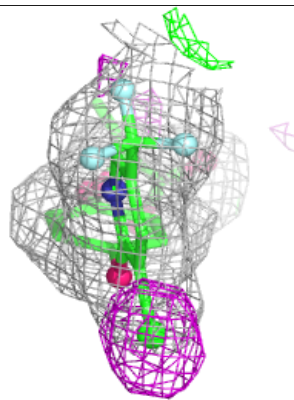
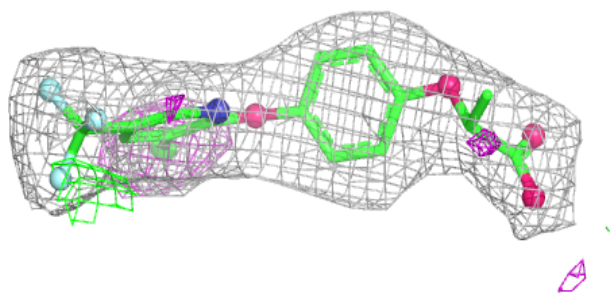
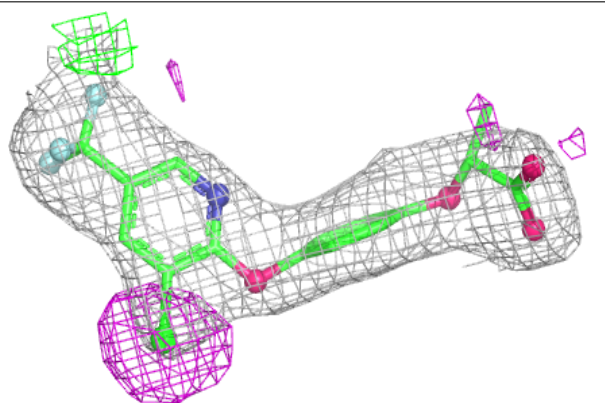


Electron density around H1L C 3000:

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

**Electron density around H1L A 3000:**

$2mF_o-DF_c$ (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.