



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

PDB ID : 1MX9
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with nalox-one methiodide, a heroin analogue
Authors : Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2002-10-01
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

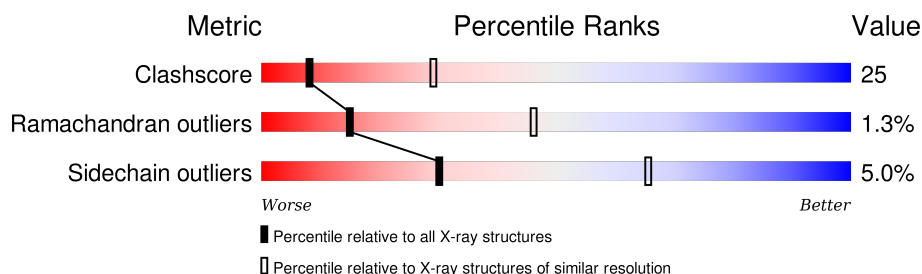
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

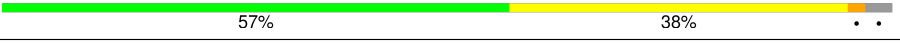




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	J	479	-	-	X	-
3	NLX	A	1	X	-	X	-
3	NLX	B	2	X	-	X	-
3	NLX	C	3	X	-	X	-
3	NLX	D	4	X	-	X	-
3	NLX	E	5	X	-	X	-
3	NLX	F	6	X	-	X	-
3	NLX	G	1	X	-	X	-
3	NLX	H	2	X	-	X	-
3	NLX	I	3	X	-	X	-
3	NLX	J	4	X	-	X	-
3	NLX	K	5	X	-	X	-
3	NLX	L	6	X	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51134 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 liver Carboxylesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	C	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	D	533	Total	C	N	O	S	0	0	0
			4135	2665	686	764	20			
1	E	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	F	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	I	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	J	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	K	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	L	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			

There are 12 discrepancies between the modelled and reference sequences:

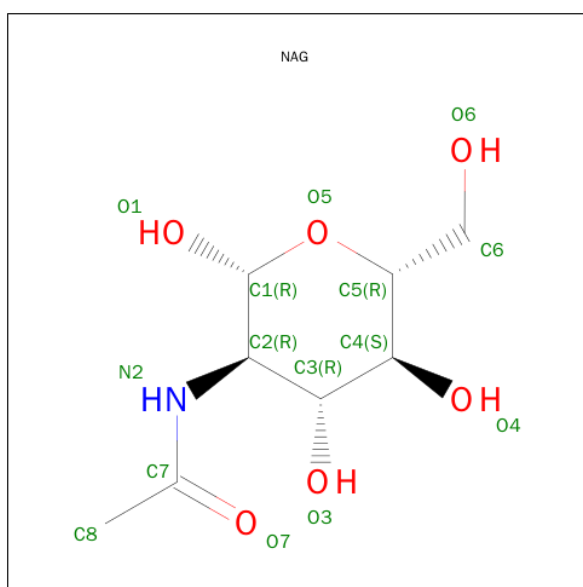
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141
D	?	-	GLN	DELETION	UNP P23141
E	?	-	GLN	DELETION	UNP P23141

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	DELETION	UNP P23141
G	?	-	GLN	DELETION	UNP P23141
H	?	-	GLN	DELETION	UNP P23141
I	?	-	GLN	DELETION	UNP P23141
J	?	-	GLN	DELETION	UNP P23141
K	?	-	GLN	DELETION	UNP P23141
L	?	-	GLN	DELETION	UNP P23141

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



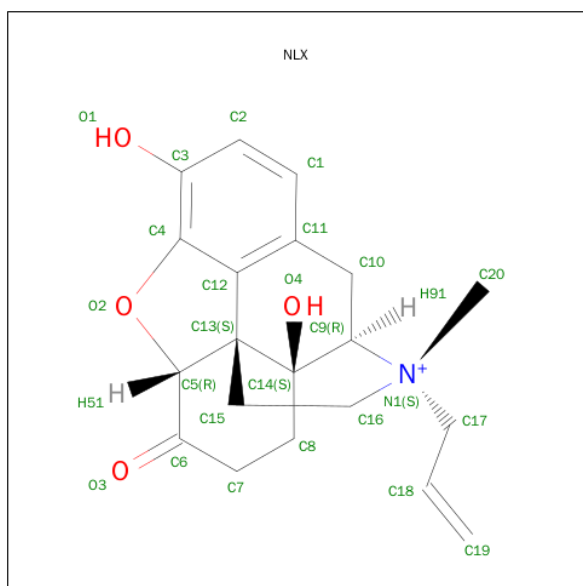
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (5A,17R)-4,5-EPOXY-3,14-DIHYDROXY-17-METHYL-6-OXO-17-(2-PROPENYL)-MORPHINANIUM (three-letter code: NLX) (formula: C₂₀H₂₄NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	20	1	4		
3	B	1	Total	C	N	O	0	0
			25	20	1	4		
3	C	1	Total	C	N	O	0	0
			25	20	1	4		
3	D	1	Total	C	N	O	0	0
			25	20	1	4		
3	E	1	Total	C	N	O	0	0
			25	20	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			25	20	1	4		
3	G	1	Total	C	N	O	0	0
			25	20	1	4		
3	H	1	Total	C	N	O	0	0
			25	20	1	4		
3	I	1	Total	C	N	O	0	0
			25	20	1	4		
3	J	1	Total	C	N	O	0	0
			25	20	1	4		
3	K	1	Total	C	N	O	0	0
			25	20	1	4		
3	L	1	Total	C	N	O	0	0
			25	20	1	4		

- Molecule 4 is water.

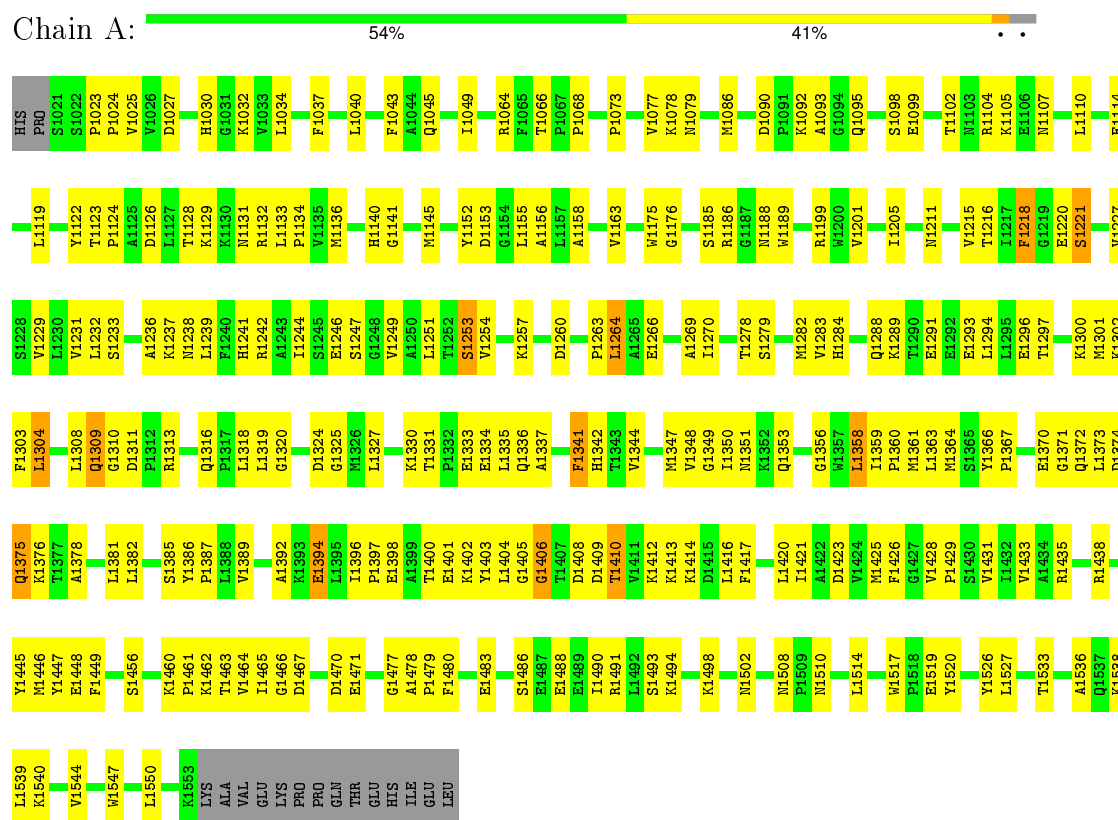
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	120	Total	O	0	0
			120	120		
4	C	98	Total	O	0	0
			98	98		
4	D	119	Total	O	0	0
			119	119		
4	E	112	Total	O	0	0
			112	112		
4	F	91	Total	O	0	0
			91	91		
4	G	69	Total	O	0	0
			69	69		
4	H	95	Total	O	0	0
			95	95		
4	I	80	Total	O	0	0
			80	80		
4	J	110	Total	O	0	0
			110	110		
4	K	73	Total	O	0	0
			73	73		
4	L	75	Total	O	0	0
			75	75		

3 Residue-property plots

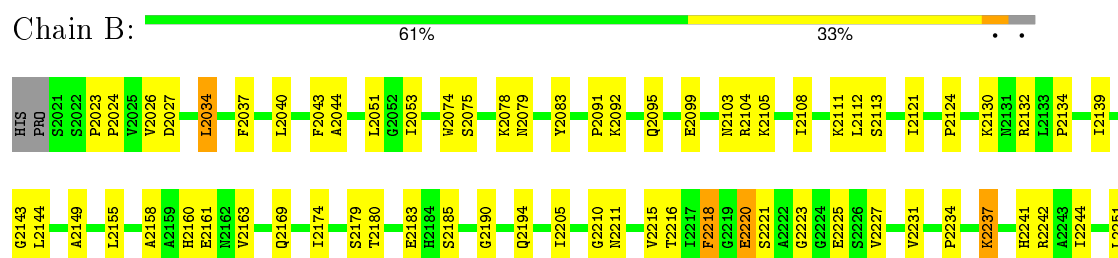
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

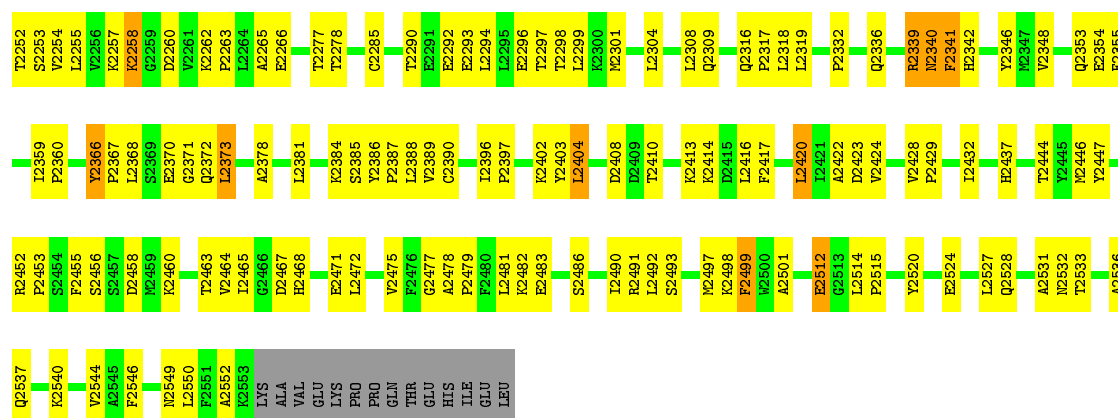
Note EDS was not executed.

- Molecule 1: liver Carboxylesterase I

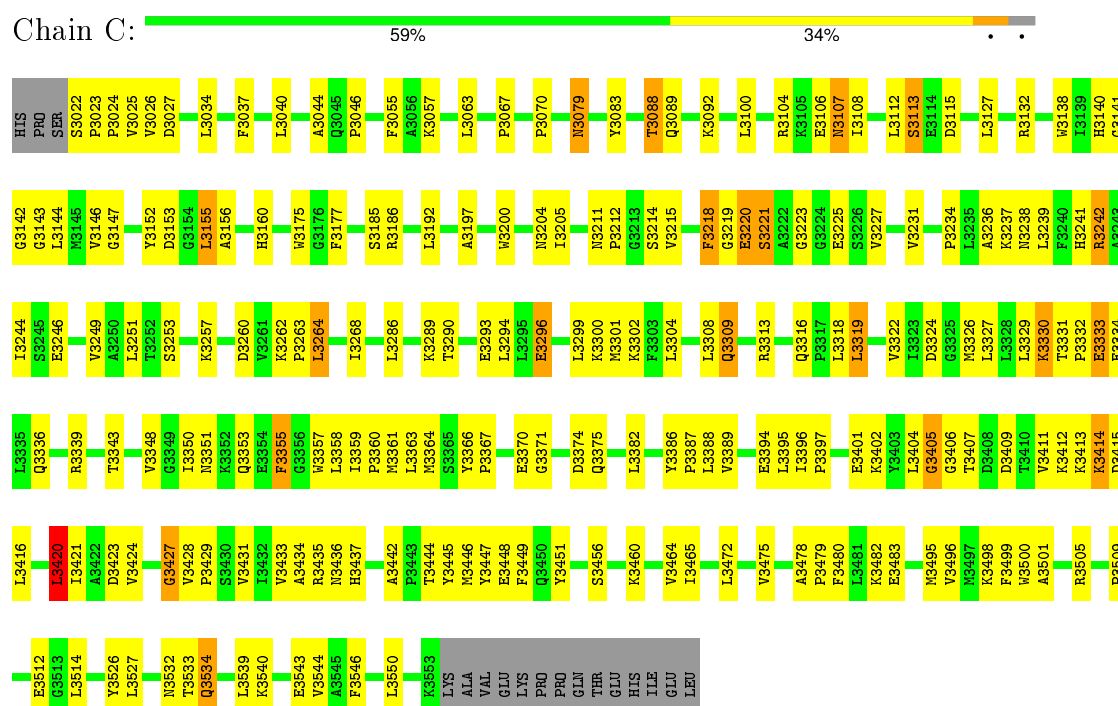


- Molecule 1: liver Carboxylesterase I

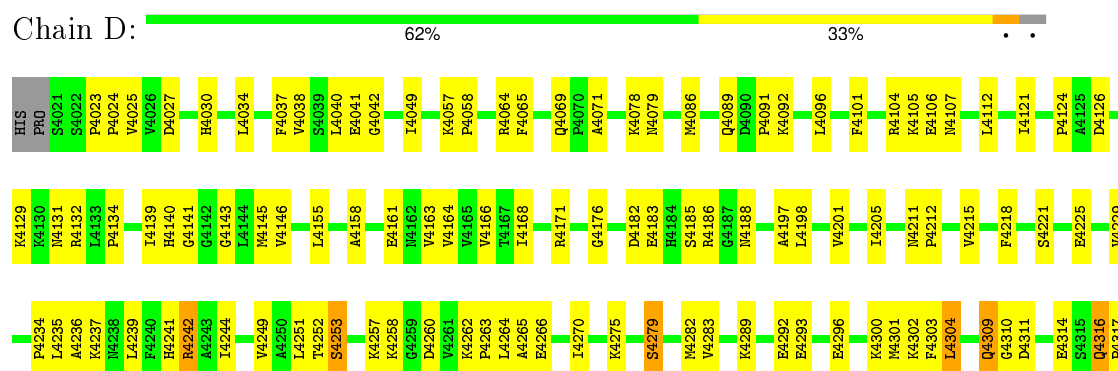


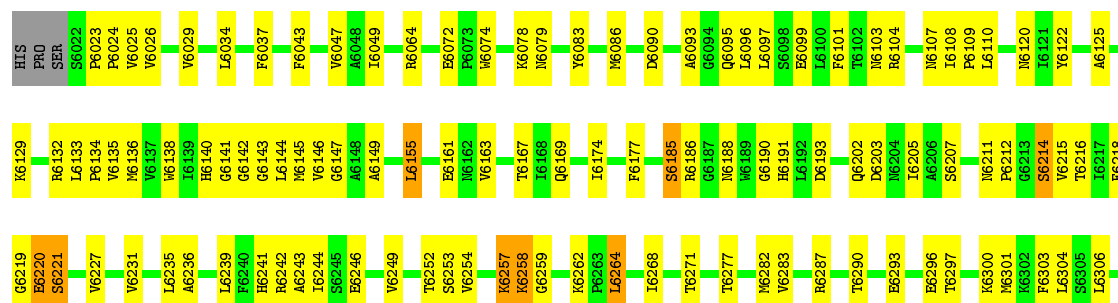


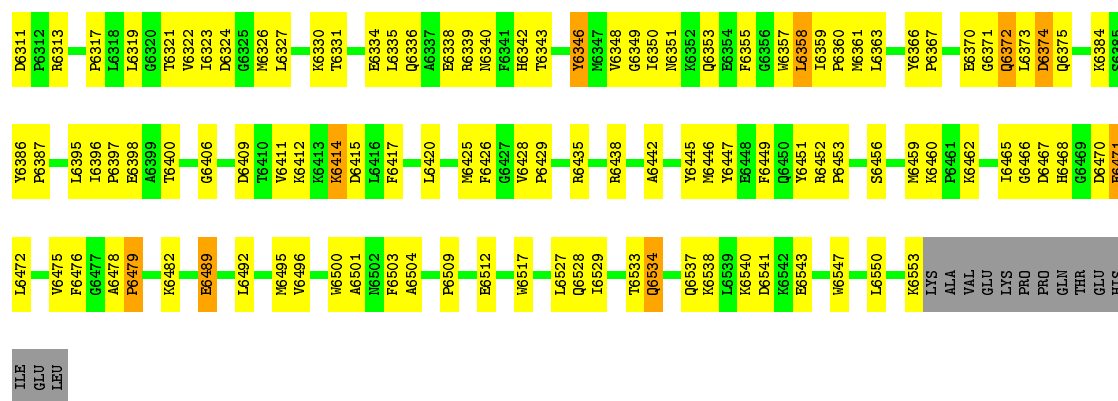
• Molecule 1: liver Carboxylesterase I



• Molecule 1: liver Carboxylesterase I

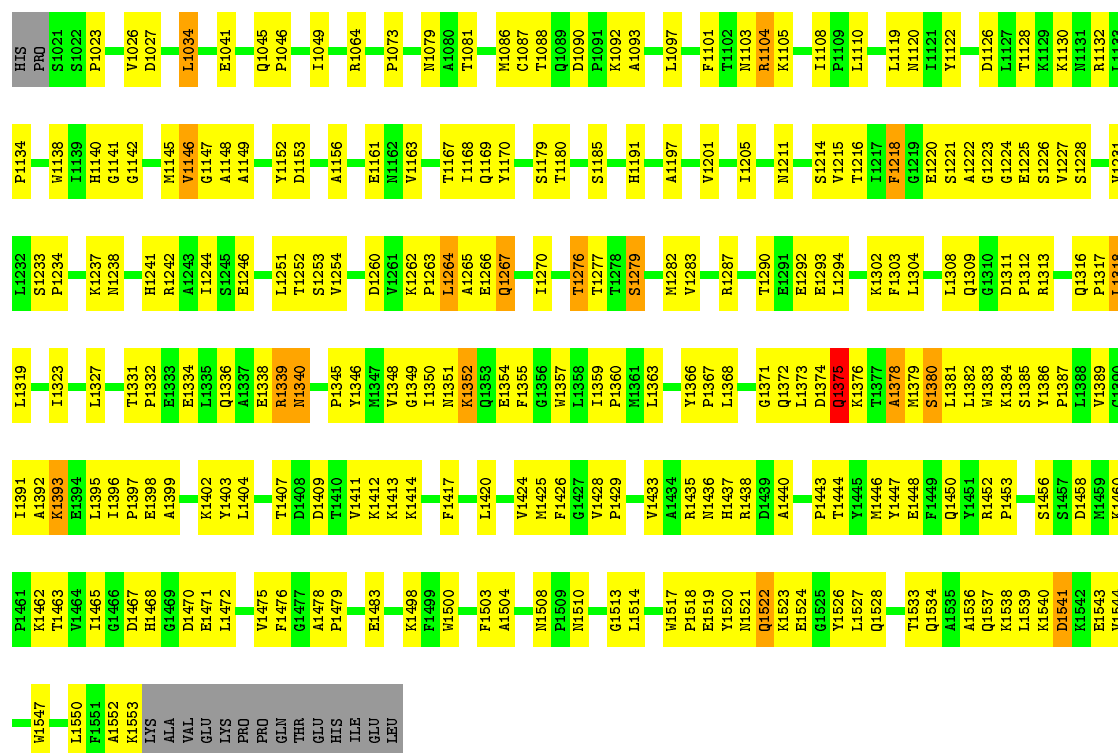






• Molecule 1: liver Carboxylesterase I

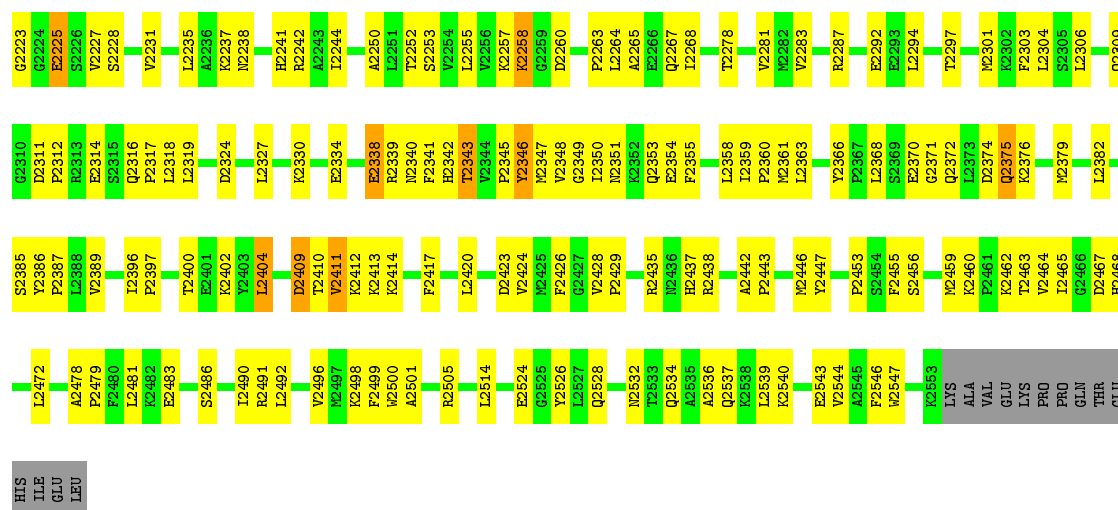
Chain G: 53% 41%



• Molecule 1: liver Carboxylesterase I

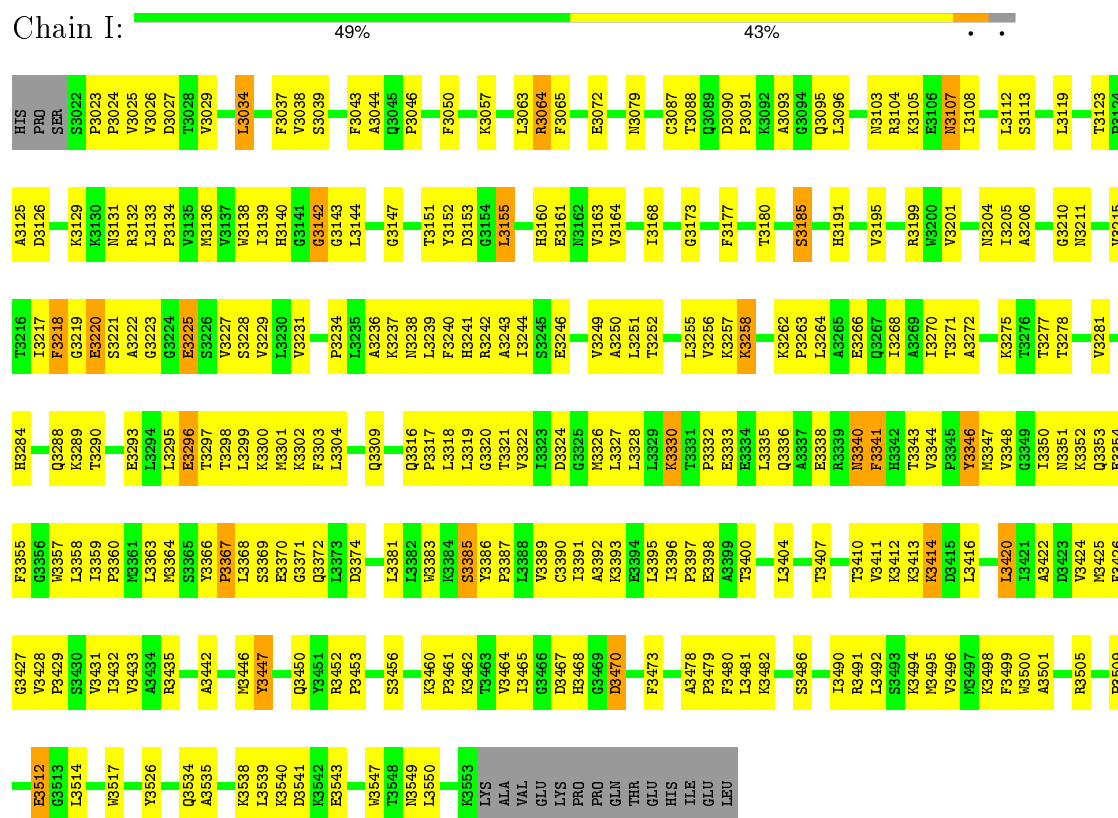
Chain H: 57% 38%





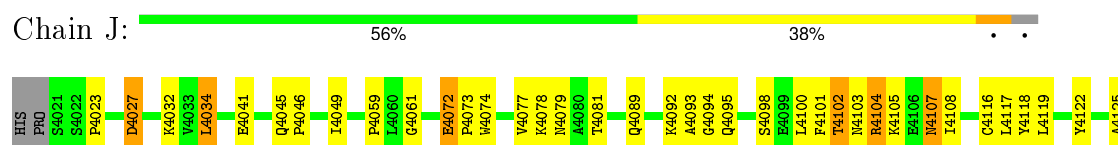
• Molecule 1: liver Carboxylesterase I

Chain I:



• Molecule 1: liver Carboxylesterase I

Chain J:





W5547	L6465	L6373	V6283	L6198	I6110
T6546	H6468	D6374	I6286	M6204	K6111
M6549		Q6375		I6205	L6112
L6550	E6471	A6378	K6289	A6206	S6113
	L6472		T6290	S6207	E6114
		L6382	E6291		D6115
	V6475	M6383	E6292	V6215	
			E6293	T6216	I6121
	A6478	Y6386		I6217	Y6122
	P6479	P6387	T6297	F6218	T6123
	F6480			G6219	P6124
	L6481	K6393	K6302	E6220	A6125
		E6394	F6303	S6221	D6126
	G6484	I6395	I6304	A6222	L6127
	A6485	I6396		G6223	T6128
	S6486		D6311	G6224	K6129
	E6487	T6400	P6312	E6225	K6130
		E6401	R6313	S6226	
				V6227	L6133
	L6492	D6409	Q6316		P6134
	S6493	T6410	P6317	S6233	V6135
		V6496	L6318	P6234	M6136
	V6496	K6412	L6319	L6235	V6137
	K6498	K6413		A6236	M6138
	F6499	K6414	V6322	K6237	I6139
	M6500	D6415	I6323	M6238	H6140
	A6501	L6416	D6324		G6141
		F6417	G6325	H6241	G6142
	A6504	L6418	M6326	R6242	G6143
		D6419	L6327		L6144
	P6509	L6420		I6244	M6145
			E6333	S6245	
	M6517	F6426		E6246	A6149
	Y6520	G6427	Q6336		L6155
		P6429		L6251	A6156
			R6339	T6252	
	K6523	I6432		S6253	E6161
	E6524	V6433	H6342	V6254	R6162
	G6525	A6434		L6255	V6163
	Y6526		M6347	V6256	
	L6527	R6435	V6348	K6257	Q6169
	Q6528		G6349	K6258	Y6170
	I6529	D6439	I6350	G6259	R6171
	G6530		M6351	D6260	
	A6531	T6444		V6261	I6174
	M6532	Y6445	F6355	K6262	M6175
	T6533	M6446	G6356	P6263	G6176
	Q6534	Y6447	M6357	L6264	F6177
	A6535		L6358	A6265	
	A6536	R6452	I6359	E6266	D6182
	Q6537	P6453	P6360	Q6267	E6183
	K6538		M6361	I6268	H6184
	L6539	S6456	L6363		S6185
	K6540			T6271	R6186
	D6541	M6459	Y6366		G6187
		K6460	P6367	T6278	M6188
	V6544			S6279	
	A6545	T6463	G6371	A6280	Q6194
	F6546	V6464	Q6372		

K6553	LYS
	ALA
	VAL
	GLU
	LYS
	PRO
	PRO
	GLN
	THR
	GLU
	HIS
	ILE
	GLU
	LEU

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.17Å 120.71Å 177.02Å 90.28° 89.32° 99.22°	Depositor
Resolution (Å)	29.82 – 2.90	Depositor
% Data completeness (in resolution range)	95.7 (29.82-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51134	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.38	0/4236	0.62	0/5754
1	B	0.41	0/4236	0.66	2/5754 (0.0%)
1	C	0.42	0/4230	0.65	2/5746 (0.0%)
1	D	0.41	0/4241	0.63	0/5761
1	E	0.40	0/4230	0.64	1/5746 (0.0%)
1	F	0.38	0/4230	0.62	0/5746
1	G	0.36	0/4236	0.60	0/5754
1	H	0.39	0/4230	0.63	0/5746
1	I	0.36	0/4230	0.61	0/5746
1	J	0.39	0/4236	0.62	0/5754
1	K	0.36	0/4230	0.60	0/5746
1	L	0.37	0/4230	0.63	1/5746 (0.0%)
All	All	0.39	0/50795	0.63	6/68999 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3420	LEU	CA-CB-CG	5.80	128.63	115.30
1	C	3388	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	B	2339	ARG	N-CA-C	5.37	125.50	111.00
1	B	2075	SER	N-CA-C	5.33	125.41	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6140	HIS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	5118	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4132	231	0
1	B	4130	0	4132	182	0
1	C	4124	0	4127	180	0
1	D	4135	0	4134	165	0
1	E	4124	0	4127	200	0
1	F	4124	0	4127	192	0
1	G	4130	0	4132	237	0
1	H	4124	0	4127	194	0
1	I	4124	0	4127	232	0
1	J	4130	0	4134	216	0
1	K	4124	0	4127	226	0
1	L	4124	0	4127	244	0
2	A	28	0	26	3	0
2	B	14	0	13	4	0
2	C	14	0	13	0	0
2	D	14	0	13	4	0
2	E	14	0	13	2	0
2	F	14	0	13	0	0
2	G	14	0	13	4	0
2	H	14	0	13	1	0
2	I	14	0	13	1	0
2	J	14	0	13	7	0
2	K	14	0	13	1	0
2	L	14	0	13	0	0
3	A	25	0	23	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	23	21	0
3	C	25	0	19	27	0
3	D	25	0	24	15	0
3	E	25	0	24	18	0
3	F	25	0	21	23	0
3	G	25	0	23	12	0
3	H	25	0	23	30	0
3	I	25	0	24	19	0
3	J	25	0	24	20	0
3	K	25	0	24	18	0
3	L	25	0	24	23	0
4	A	87	0	0	9	0
4	B	120	0	0	12	0
4	C	98	0	0	10	0
4	D	119	0	0	9	0
4	E	112	0	0	16	0
4	F	91	0	0	8	0
4	G	69	0	0	10	0
4	H	95	0	0	10	0
4	I	80	0	0	10	0
4	J	110	0	0	8	0
4	K	73	0	0	11	0
4	L	75	0	0	15	0
All	All	51134	0	49998	2453	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 25.

The worst 5 of 2453 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)
3:C:3:NLX:N1	3:C:3:NLX:C9	1.69	1.56
3:C:3:NLX:C9	3:C:3:NLX:C14	1.78	1.55
1:D:4343:THR:HB	1:D:4442:ALA:HB2	1.17	1.13
1:H:2304:LEU:HB3	3:H:2:NLX:H201	1.28	1.11
1:C:3364:MET:CE	3:C:3:NLX:H181	1.83	1.08

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	530/548 (97%)	480 (91%)	41 (8%)	9 (2%)	11	38
1	B	530/548 (97%)	476 (90%)	48 (9%)	6 (1%)	17	51
1	C	529/548 (96%)	489 (92%)	33 (6%)	7 (1%)	15	46
1	D	531/548 (97%)	491 (92%)	36 (7%)	4 (1%)	24	60
1	E	529/548 (96%)	482 (91%)	40 (8%)	7 (1%)	15	46
1	F	529/548 (96%)	477 (90%)	44 (8%)	8 (2%)	13	42
1	G	530/548 (97%)	467 (88%)	55 (10%)	8 (2%)	13	42
1	H	529/548 (96%)	470 (89%)	52 (10%)	7 (1%)	15	46
1	I	529/548 (96%)	466 (88%)	56 (11%)	7 (1%)	15	46
1	J	530/548 (97%)	484 (91%)	40 (8%)	6 (1%)	17	51
1	K	529/548 (96%)	475 (90%)	48 (9%)	6 (1%)	17	51
1	L	529/548 (96%)	467 (88%)	53 (10%)	9 (2%)	11	38
All	All	6354/6576 (97%)	5724 (90%)	546 (9%)	84 (1%)	15	46

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	SER
1	B	2342	HIS
1	C	3253	SER
1	D	4185	SER
1	D	4253	SER

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	448/463 (97%)	435 (97%)	13 (3%)	50	83
1	B	448/463 (97%)	431 (96%)	17 (4%)	40	76
1	C	447/463 (96%)	420 (94%)	27 (6%)	24	57
1	D	448/463 (97%)	423 (94%)	25 (6%)	26	60
1	E	447/463 (96%)	422 (94%)	25 (6%)	26	60
1	F	447/463 (96%)	426 (95%)	21 (5%)	32	68
1	G	448/463 (97%)	419 (94%)	29 (6%)	21	52
1	H	447/463 (96%)	427 (96%)	20 (4%)	34	70
1	I	447/463 (96%)	418 (94%)	29 (6%)	21	52
1	J	448/463 (97%)	426 (95%)	22 (5%)	31	67
1	K	447/463 (96%)	421 (94%)	26 (6%)	25	58
1	L	447/463 (96%)	433 (97%)	14 (3%)	47	82
All	All	5369/5556 (97%)	5101 (95%)	268 (5%)	30	65

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	6374	ASP
1	G	1393	LYS
1	K	5426	PHE
1	F	6489	GLU
1	G	1226	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	5506	ASN
1	G	1140	HIS
1	K	5351	ASN
1	E	5537	GLN
1	F	6241	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

25 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	NLX	A	1	-	26,29,29	3.43	16 (61%)	38,49,49	1.85	11 (28%)
2	NAG	A	179	-	14,14,15	0.62	0	15,19,21	0.74	0
2	NAG	A	180	-	14,14,15	0.58	0	15,19,21	0.74	1 (6%)
3	NLX	B	2	-	26,29,29	2.79	15 (57%)	38,49,49	1.74	9 (23%)
2	NAG	B	279	-	14,14,15	0.47	0	15,19,21	0.65	0
3	NLX	C	3	-	26,29,29	4.12	17 (65%)	38,49,49	5.43	15 (39%)
2	NAG	C	379	-	14,14,15	0.46	0	15,19,21	0.77	0
3	NLX	D	4	-	26,29,29	3.08	15 (57%)	38,49,49	1.91	13 (34%)
2	NAG	D	479	-	14,14,15	0.44	0	15,19,21	0.69	1 (6%)
3	NLX	E	5	-	26,29,29	2.89	15 (57%)	38,49,49	1.80	10 (26%)
2	NAG	E	579	-	14,14,15	0.49	0	15,19,21	0.83	1 (6%)
3	NLX	F	6	-	26,29,29	3.23	16 (61%)	38,49,49	5.35	17 (44%)
2	NAG	F	679	-	14,14,15	0.49	0	15,19,21	0.82	1 (6%)
3	NLX	G	1	-	26,29,29	3.18	15 (57%)	38,49,49	1.85	10 (26%)
2	NAG	G	179	-	14,14,15	0.55	0	15,19,21	0.67	0
3	NLX	H	2	-	26,29,29	3.06	14 (53%)	38,49,49	1.98	11 (28%)
2	NAG	H	279	-	14,14,15	0.47	0	15,19,21	0.69	0
3	NLX	I	3	-	26,29,29	2.95	16 (61%)	38,49,49	1.93	11 (28%)
2	NAG	I	379	-	14,14,15	0.46	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NLX	J	4	-	26,29,29	3.18	14 (53%)	38,49,49	1.71	9 (23%)
2	NAG	J	479	-	14,14,15	0.54	0	15,19,21	0.71	1 (6%)
3	NLX	K	5	-	26,29,29	2.97	14 (53%)	38,49,49	1.76	10 (26%)
2	NAG	K	579	-	14,14,15	0.51	0	15,19,21	0.82	1 (6%)
3	NLX	L	6	-	26,29,29	3.15	15 (57%)	38,49,49	1.86	11 (28%)
2	NAG	L	679	-	14,14,15	0.59	0	15,19,21	0.72	1 (6%)

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	NLX	A	1	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	A	179	-	-	0/6/23/26	0/1/1/1
2	NAG	A	180	-	-	0/6/23/26	0/1/1/1
3	NLX	B	2	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	B	279	-	-	0/6/23/26	0/1/1/1
3	NLX	C	3	-	1/1/6/7	1/4/62/62	0/3/5/5
2	NAG	C	379	-	-	0/6/23/26	0/1/1/1
3	NLX	D	4	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	D	479	-	-	0/6/23/26	0/1/1/1
3	NLX	E	5	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	E	579	-	-	0/6/23/26	0/1/1/1
3	NLX	F	6	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	F	679	-	-	0/6/23/26	0/1/1/1
3	NLX	G	1	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	G	179	-	-	0/6/23/26	0/1/1/1
3	NLX	H	2	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	H	279	-	-	0/6/23/26	0/1/1/1
3	NLX	I	3	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	I	379	-	-	0/6/23/26	0/1/1/1
3	NLX	J	4	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	J	479	-	-	0/6/23/26	0/1/1/1
3	NLX	K	5	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	K	579	-	-	0/6/23/26	0/1/1/1
3	NLX	L	6	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	L	679	-	-	0/6/23/26	0/1/1/1

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	NLX	C13-C12	2.01	1.54	1.50
3	K	5	NLX	C1-C11	2.03	1.43	1.39
3	E	5	NLX	C13-C12	2.05	1.54	1.50
3	K	5	NLX	C2-C3	2.05	1.43	1.39
3	G	1	NLX	C2-C3	2.05	1.43	1.39

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NLX	C20-N1-C17	-24.38	63.74	108.74
3	F	6	NLX	C20-N1-C17	-23.08	66.14	108.74
3	C	3	NLX	C20-N1-C16	-17.31	68.71	108.68
3	F	6	NLX	C20-N1-C16	-15.98	71.79	108.68
3	H	2	NLX	C8-C14-C13	-4.32	107.38	111.33

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	NLX	N1
3	K	5	NLX	N1
3	L	6	NLX	N1
3	J	4	NLX	N1
3	F	6	NLX	N1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	NLX	C19-C18-C17-N1

There are no ring outliers.

22 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NLX	20	0
2	A	179	NAG	3	0
2	A	180	NAG	1	0
3	B	2	NLX	21	0
2	B	279	NAG	4	0
3	C	3	NLX	27	0
3	D	4	NLX	15	0
2	D	479	NAG	4	0
3	E	5	NLX	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	579	NAG	2	0
3	F	6	NLX	23	0
3	G	1	NLX	12	0
2	G	179	NAG	4	0
3	H	2	NLX	30	0
2	H	279	NAG	1	0
3	I	3	NLX	19	0
2	I	379	NAG	1	0
3	J	4	NLX	20	0
2	J	479	NAG	7	0
3	K	5	NLX	18	0
2	K	579	NAG	1	0
3	L	6	NLX	23	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.