



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:59 PM GMT

PDB ID : 1MX5
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with homatropine, a cocaine analogue
Authors : Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2002-10-01
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
<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

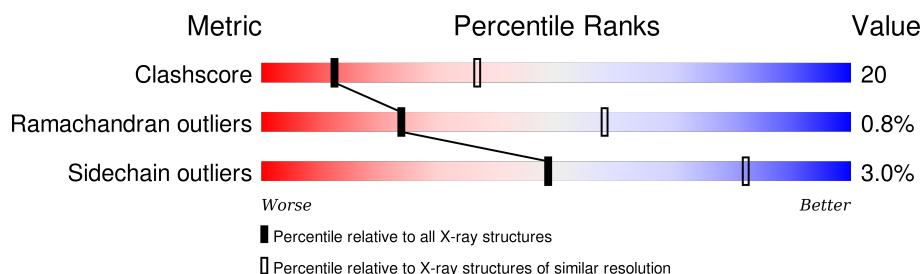
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 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	

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
4	SIA	B	282	-	-	X	-
5	CL	A	11	-	-	X	-
5	CL	E	15	-	-	X	-
6	HTQ	A	111	-	-	X	-
6	HTQ	B	212	-	-	X	-
6	HTQ	E	515	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26960 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.

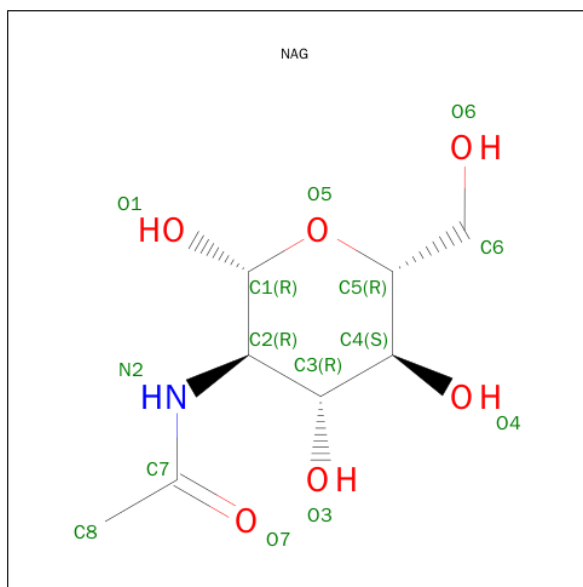
- Molecule 1 is a protein called liver Carboxylesterase I.

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	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	C	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	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			

There are 6 discrepancies between the modelled and reference sequences:

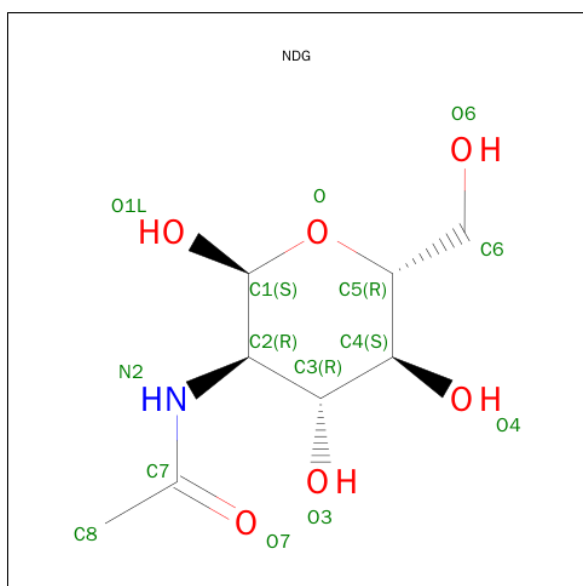
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141
D	?	-	GLN	DELETION	UNP P23141
E	?	-	GLN	DELETION	UNP P23141
F	?	-	GLN	DELETION	UNP P23141

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



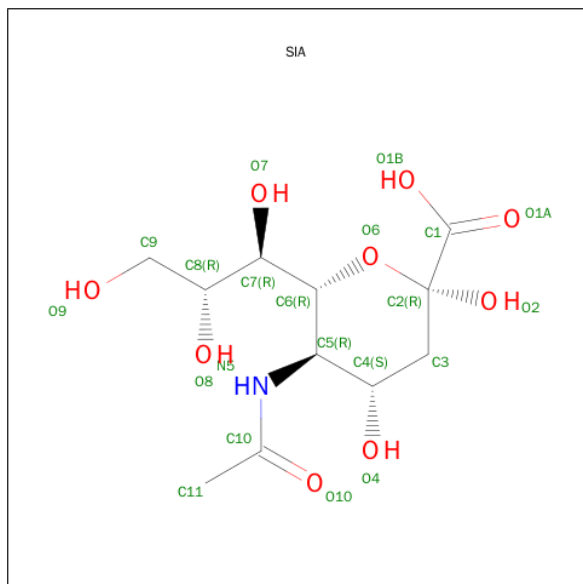
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).

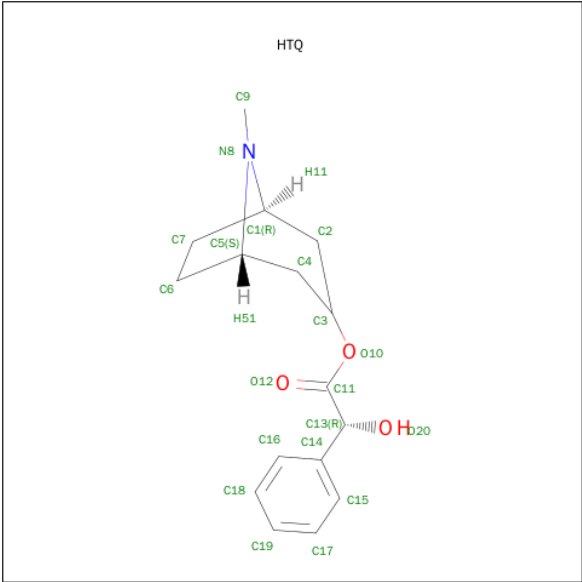


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	11	1	9		
4	B	1	Total	C	N	O	0	0
			21	11	1	9		
4	F	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		

- Molecule 6 is HOMOTROPINE (three-letter code: HTQ) (formula: $C_{16}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	16	1	3		
6	B	1	Total	C	N	O	0	0
			20	16	1	3		
6	C	1	Total	C	N	O	0	0
			20	16	1	3		
6	D	1	Total	C	N	O	0	0
			20	16	1	3		
6	E	1	Total	C	N	O	0	0
			20	16	1	3		
6	F	1	Total	C	N	O	0	0
			20	16	1	3		
6	A	1	Total	C	N	O	0	1
			40	32	2	6		
6	B	1	Total	C	N	O	0	1
			40	32	2	6		
6	C	1	Total	C	N	O	0	1
			40	32	2	6		
6	D	1	Total	C	N	O	0	1
			40	32	2	6		
6	E	1	Total	C	N	O	0	1
			40	32	2	6		
6	F	1	Total	C	N	O	0	1
			40	32	2	6		

- Molecule 7 is water.

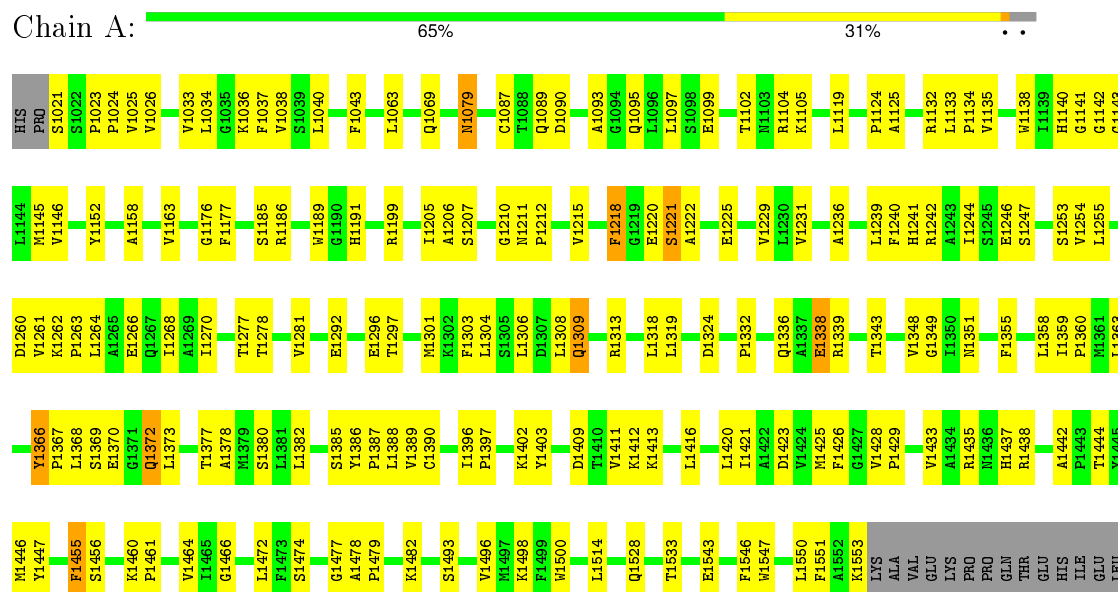
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	249	Total 249	O 249	0	0
7	B	303	Total 303	O 303	0	0
7	C	289	Total 289	O 289	0	0
7	D	291	Total 291	O 291	0	0
7	E	295	Total 295	O 295	0	0
7	F	254	Total 254	O 254	0	0

3 Residue-property plots

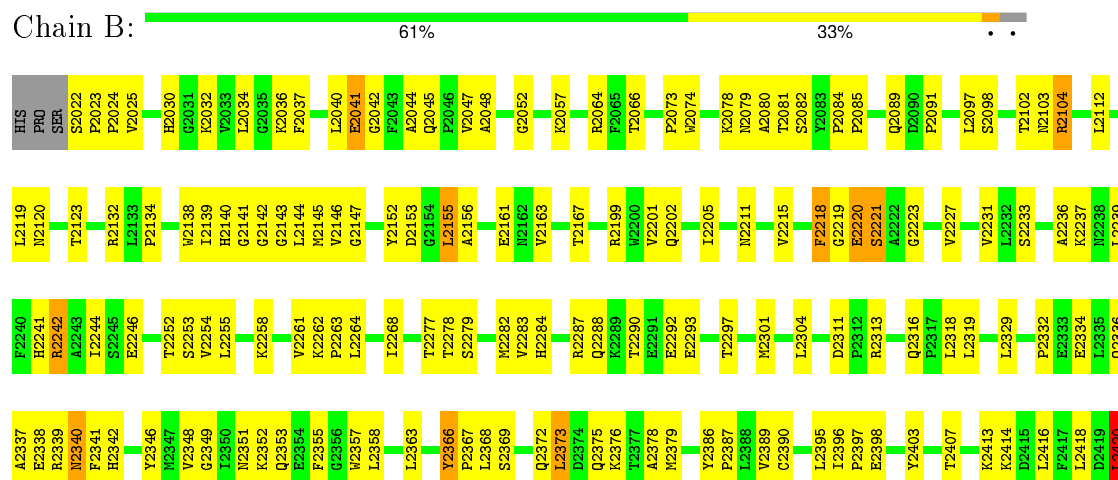
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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





PRO
PRO
GLN
THR
GLU
HIS
ILE
GLU
LEU

• Molecule 1: liver Carboxylesterase I

Chain E:  62% 32%

A5552	H5553	N5540	V5541	F5542	T5543	V5544	V5548	G5549	N5551	E5554	F5555	G5556	H5557	L5558	T5559	P5560	M5561	L5563	M5564	S5565	P5567	L5568	L5581	L5582	E5583	K5584	S5585	S5586	P5587	L5588	L5591	L5592	L5594	L5595	T5596	P5597	K5602	F5603	L5604	S5605	L5606	D5611	P5612	R5613	E5614	S5615	Q5616	P5617	L5618	L5619	L5628	P5629	D5630	V5631	K5632	P5633	L5634	Q5635	T5636	P5637	L5638	L5647	H5648	L5649	F5650	E5651	L5652	L5653	L5654	L5655	L5656	L5657	L5658	L5659	L5660	L5661	L5662	L5663	L5664	L5665	L5666	L5667	L5668	L5669	L5670	L5671	L5672	L5673	L5674	L5675	L5676	L5677	L5678	L5679	L5680	L5681	L5682	L5683	L5684	L5685	L5686	L5687	L5688	L5689	L5690	L5691	L5692	L5693	L5694	L5695	L5696	L5697	L5698	L5699	L5700	L5701	L5702	L5703	L5704	L5705	L5706	L5707	L5708	L5709	L5710	L5711	L5712	L5713	L5714	L5715	L5716	L5717	L5718	L5719	L5720	L5721	L5722	L5723	L5724	L5725	L5726	L5727	L5728	L5729	L5730	L5731	L5732	L5733	L5734	L5735	L5736	L5737	L5738	L5739	L5740	L5741	L5742	L5743	L5744	L5745	L5746	L5747	L5748	L5749	L5750	L5751	L5752	L5753	L5754	L5755	L5756	L5757	L5758	L5759	L5760	L5761	L5762	L5763	L5764	L5765	L5766	L5767	L5768	L5769	L5770	L5771	L5772	L5773	L5774	L5775	L5776	L5777	L5778	L5779	L5780	L5781	L5782	L5783	L5784	L5785	L5786	L5787	L5788	L5789	L5790	L5791	L5792	L5793	L5794	L5795	L5796	L5797	L5798	L5799	L5800	L5801	L5802	L5803	L5804	L5805	L5806	L5807	L5808	L5809	L5810	L5811	L5812	L5813	L5814	L5815	L5816	L5817	L5818	L5819	L5820	L5821	L5822	L5823	L5824	L5825	L5826	L5827	L5828	L5829	L5830	L5831	L5832	L5833	L5834	L5835	L5836	L5837	L5838	L5839	L5840	L5841	L5842	L5843	L5844	L5845	L5846	L5847	L5848	L5849	L5850	L5851	L5852	L5853	L5854	L5855	L5856	L5857	L5858	L5859	L5860	L5861	L5862	L5863	L5864	L5865	L5866	L5867	L5868	L5869	L5870	L5871	L5872	L5873	L5874	L5875	L5876	L5877	L5878	L5879	L5880	L5881	L5882	L5883	L5884	L5885	L5886	L5887	L5888	L5889	L5890	L5891	L5892	L5893	L5894	L5895	L5896	L5897	L5898	L5899	L5900	L5901	L5902	L5903	L5904	L5905	L5906	L5907	L5908	L5909	L5910	L5911	L5912	L5913	L5914	L5915	L5916	L5917	L5918	L5919	L5920	L5921	L5922	L5923	L5924	L5925	L5926	L5927	L5928	L5929	L5930	L5931	L5932	L5933	L5934	L5935	L5936	L5937	L5938	L5939	L5940	L5941	L5942	L5943	L5944	L5945	L5946	L5947	L5948	L5949	L5950	L5951	L5952	L5953	L5954	L5955	L5956	L5957	L5958	L5959	L5960	L5961	L5962	L5963	L5964	L5965	L5966	L5967	L5968	L5969	L5970	L5971	L5972	L5973	L5974	L5975	L5976	L5977	L5978	L5979	L5980	L5981	L5982	L5983	L5984	L5985	L5986	L5987	L5988	L5989	L5990	L5991	L5992	L5993	L5994	L5995	L5996	L5997	L5998	L5999	L6000	L6001	L6002	L6003	L6004	L6005	L6006	L6007	L6008	L6009	L6010	L6011	L6012	L6013	L6014	L6015	L6016	L6017	L6018	L6019	L6020	L6021	L6022	L6023	L6024	L6025	L6026	L6027	L6028	L6029	L6030	L6031	L6032	L6033	L6034	L6035	L6036	L6037	L6038	L6039	L6040	L6041	L6042	L6043	L6044	L6045	L6046	L6047	L6048	L6049	L6050	L6051	L6052	L6053	L6054	L6055	L6056	L6057	L6058	L6059	L6060	L6061	L6062	L6063	L6064	L6065	L6066	L6067	L6068	L6069	L6070	L6071	L6072	L6073	L6074	L6075	L6076	L6077	L6078	L6079	L6080	L6081	L6082	L6083	L6084	L6085	L6086	L6087	L6088	L6089	L6090	L6091	L6092	L6093	L6094	L6095	L6096	L6097	L6098	L6099	L6100	L6101	L6102	L6103	L6104	L6105	L6106	L6107	L6108	L6109	L6110	L6111	L6112	L6113	L6114	L6115	L6116	L6117	L6118	L6119	L6120	L6121	L6122	L6123	L6124	L6125	L6126	L6127	L6128	L6129	L6130	L6131	L6132	L6133	L6134	L6135	L6136	L6137	L6138	L6139	L6140	L6141	L6142	L6143	L6144	L6145	L6146	L6147	L6148	L6149	L6150	L6151	L6152	L6153	L6154	L6155	L6156	L6157	L6158	L6159	L6160	L6161	L6162	L6163	L6164	L6165	L6166	L6167	L6168	L6169	L6170	L6171	L6172	L6173	L6174	L6175	L6176	L6177	L6178	L6179	L6180	L6181	L6182	L6183	L6184	L6185	L6186	L6187	L6188	L6189	L6190	L6191	L6192	L6193	L6194	L6195	L6196	L6197	L6198	L6199	L6200	L6201	L6202	L6203	L6204	L6205	L6206	L6207	L6208	L6209	L6210	L6211	L6212	L6213	L6214	L6215	L6216	L6217	L6218	L6219	L6220	L6221	L6222	L6223	L6224	L6225	L6226	L6227	L6228	L6229	L6230	L6231	L6232	L6233	L6234	L6235	L6236	L6237	L6238	L6239	L6240	L6241	L6242	L6243	L6244	L6245	L6246	L6247	L6248	L6249	L6250	L6251	L6252	L6253	L6254	L6255	L6256	L6257	L6258	L6259	L6260	L6261	L6262	L6263	L6264	L6265	L6266	L6267	L6268	L6269	L6270	L6271	L6272	L6273	L6274	L6275	L6276	L6277	L6278	L6279	L6280	L6281	L6282	L6283	L6284	L6285	L6286	L6287	L6288	L6289	L6290	L6291	L6292	L6293	L6294	L6295	L6296	L6297	L6298	L6299	L6300	L6301	L6302	L6303	L6304	L6305	L6306	L6307	L6308	L6309	L6310	L6311	L6312	L6313	L6314	L6315	L6316	L6317	L6318	L6319	L6320	L6321	L6322	L6323	L6324	L6325	L6326	L6327	L6328	L6329	L6330	L6331	L6332	L6333	L6334	L6335	L6336	L6337	L6338	L6339	L6340	L6341	L6342	L6343	L6344	L6345	L6346	L6347	L6348	L6349	L6350	L6351	L6352	L6353	L6354	L6355	L6356	L6357	L6358	L6359	L6360	L6361	L6362	L6363	L6364	L6365	L6366	L6367	L6368	L6369	L6370	L6371	L6372	L6373	L6374	L6375	L6376	L6377	L6378	L6379	L6380	L6381	L6382	L6383	L6384	L6385	L6386	L6387	L6388	L6389	L6390	L6391	L6392	L6393	L6394	L6395	L6396	L6397	L6398	L6399	L6400	L6401	L6402	L6403	L6404	L6405	L6406	L6407	L6408	L6409	L6410	L6411	L6412	L6413	L6414	L6415	L6416	L6417	L6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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 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.40 Å 178.80 Å 199.60 Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80	Depositor
% Data completeness (in resolution range)	92.3 (19.96-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.158 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26960	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: HTQ, SIA, NAG, NDG, CL

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	0.33	0/4236	0.57	0/5754
1	B	0.34	0/4230	0.59	1/5746 (0.0%)
1	C	0.34	0/4230	0.58	0/5746
1	D	0.34	0/4236	0.59	1/5754 (0.0%)
1	E	0.33	0/4230	0.60	0/5746
1	F	0.33	0/4230	0.58	0/5746
All	All	0.34	0/25392	0.58	2/34492 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2420	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	4420	LEU	CA-CB-CG	5.05	126.91	115.30

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	4130	0	4131	161	0
1	B	4124	0	4126	181	0
1	C	4124	0	4126	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4130	0	4131	137	0
1	E	4124	0	4126	178	0
1	F	4124	0	4126	152	0
2	A	14	0	13	0	0
2	C	14	0	13	0	0
2	E	28	0	26	2	0
3	B	14	0	13	3	0
3	D	14	0	13	2	0
3	F	14	0	13	3	0
4	A	21	0	18	5	0
4	B	21	0	18	17	0
4	F	21	0	18	5	0
5	A	1	0	0	5	0
5	E	1	0	0	2	0
6	A	60	0	63	21	0
6	B	60	0	63	14	0
6	C	60	0	63	11	0
6	D	60	0	63	12	0
6	E	60	0	63	15	0
6	F	60	0	63	13	0
7	A	249	0	0	13	0
7	B	303	0	0	26	0
7	C	289	0	0	27	0
7	D	291	0	0	15	0
7	E	295	0	0	20	0
7	F	254	0	0	25	0
All	All	26960	0	25289	991	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 20.

The worst 5 of 991 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:E:5221:SER:HB3	5:E:15:CL:CL	1.58	1.39
1:F:6258:LYS:H	1:F:6258:LYS:HE2	1.17	1.08
1:C:3258:LYS:H	1:C:3258:LYS:HE2	1.19	1.02
1:B:2304:LEU:HD13	6:B:212:HTQ:H171	1.39	1.01
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.43	1.00

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	530/548 (97%)	495 (93%)	33 (6%)	2 (0%)	39	74
1	B	529/548 (96%)	496 (94%)	28 (5%)	5 (1%)	21	55
1	C	529/548 (96%)	488 (92%)	38 (7%)	3 (1%)	30	65
1	D	530/548 (97%)	503 (95%)	23 (4%)	4 (1%)	24	58
1	E	529/548 (96%)	495 (94%)	27 (5%)	7 (1%)	15	44
1	F	529/548 (96%)	493 (93%)	32 (6%)	4 (1%)	24	58
All	All	3176/3288 (97%)	2970 (94%)	181 (6%)	25 (1%)	24	58

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2253	SER
1	C	3237	LYS
1	E	5393	LYS
1	E	5462	LYS
1	F	6341	PHE

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	448/463 (97%)	437 (98%)	11 (2%)	55	86
1	B	447/463 (96%)	433 (97%)	14 (3%)	47	81
1	C	447/463 (96%)	432 (97%)	15 (3%)	44	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	448/463 (97%)	437 (98%)	11 (2%)	55	86
1	E	447/463 (96%)	431 (96%)	16 (4%)	42	76
1	F	447/463 (96%)	433 (97%)	14 (3%)	47	81
All	All	2684/2778 (97%)	2603 (97%)	81 (3%)	48	82

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3375	GLN
1	D	4309	GLN
1	F	6318	LEU
1	C	3381	LEU
1	D	4079	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3450	GLN
1	D	4241	HIS
1	F	6351	ASN
1	C	3528	GLN
1	D	4069	GLN

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

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 for Mogul analysis.

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
6	HTQ	A	1[Y]	-	22,22,22	2.11	10 (45%)	31,31,31	1.51	3 (9%)
6	HTQ	A	1[Z]	-	22,22,22	2.13	10 (45%)	31,31,31	1.80	3 (9%)
6	HTQ	A	111	-	22,22,22	1.93	8 (36%)	31,31,31	1.75	5 (16%)
2	NAG	A	179	1	14,14,15	0.61	0	15,19,21	0.78	1 (6%)
4	SIA	A	182	-	17,21,21	0.99	1 (5%)	19,31,31	1.10	2 (10%)
6	HTQ	B	2[Y]	-	22,22,22	1.99	8 (36%)	31,31,31	1.24	2 (6%)
6	HTQ	B	2[Z]	-	22,22,22	2.01	8 (36%)	31,31,31	1.40	3 (9%)
6	HTQ	B	212	-	22,22,22	1.89	7 (31%)	31,31,31	1.66	3 (9%)
3	NDG	B	279	1	14,14,15	0.51	0	15,19,21	0.77	1 (6%)
4	SIA	B	282	-	17,21,21	1.14	1 (5%)	19,31,31	1.17	1 (5%)
6	HTQ	C	3[Y]	-	22,22,22	2.03	8 (36%)	31,31,31	1.52	5 (16%)
6	HTQ	C	3[Z]	-	22,22,22	2.08	8 (36%)	31,31,31	1.50	5 (16%)
6	HTQ	C	313	-	22,22,22	2.03	8 (36%)	31,31,31	1.46	2 (6%)
2	NAG	C	379	1	14,14,15	0.55	0	15,19,21	0.71	1 (6%)
6	HTQ	D	4[Y]	-	22,22,22	2.01	8 (36%)	31,31,31	1.46	4 (12%)
6	HTQ	D	4[Z]	-	22,22,22	1.95	8 (36%)	31,31,31	1.28	2 (6%)
6	HTQ	D	414	-	22,22,22	2.07	9 (40%)	31,31,31	2.04	4 (12%)
3	NDG	D	479	1	14,14,15	0.51	0	15,19,21	0.69	1 (6%)
6	HTQ	E	5[Y]	-	22,22,22	2.04	8 (36%)	31,31,31	1.34	4 (12%)
6	HTQ	E	5[Z]	-	22,22,22	2.06	9 (40%)	31,31,31	1.50	2 (6%)
6	HTQ	E	515	-	22,22,22	2.01	8 (36%)	31,31,31	1.48	2 (6%)
2	NAG	E	579	1	14,14,15	0.55	0	15,19,21	0.74	1 (6%)
2	NAG	E	580	-	14,14,15	0.53	0	15,19,21	0.72	1 (6%)
6	HTQ	F	6[Y]	-	22,22,22	2.06	8 (36%)	31,31,31	1.42	2 (6%)
6	HTQ	F	6[Z]	-	22,22,22	2.07	9 (40%)	31,31,31	1.52	3 (9%)
6	HTQ	F	616	-	22,22,22	1.90	8 (36%)	31,31,31	1.39	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDG	F	679	1	14,14,15	0.59	0	15,19,21	0.72	1 (6%)
4	SIA	F	682	-	17,21,21	1.00	1 (5%)	19,31,31	0.77	0

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
6	HTQ	A	1[Y]	-	-	0/12/33/33	0/1/3/3
6	HTQ	A	1[Z]	-	-	0/12/33/33	0/1/3/3
6	HTQ	A	111	-	-	0/12/33/33	0/1/3/3
2	NAG	A	179	1	-	0/6/23/26	0/1/1/1
4	SIA	A	182	-	-	0/14/38/38	0/1/1/1
6	HTQ	B	2[Y]	-	-	0/12/33/33	0/1/3/3
6	HTQ	B	2[Z]	-	-	0/12/33/33	0/1/3/3
6	HTQ	B	212	-	-	0/12/33/33	0/1/3/3
3	NDG	B	279	1	-	0/6/23/26	0/1/1/1
4	SIA	B	282	-	-	0/14/38/38	0/1/1/1
6	HTQ	C	3[Y]	-	-	0/12/33/33	0/1/3/3
6	HTQ	C	3[Z]	-	-	0/12/33/33	0/1/3/3
6	HTQ	C	313	-	-	0/12/33/33	0/1/3/3
2	NAG	C	379	1	-	0/6/23/26	0/1/1/1
6	HTQ	D	4[Y]	-	-	0/12/33/33	0/1/3/3
6	HTQ	D	4[Z]	-	-	0/12/33/33	0/1/3/3
6	HTQ	D	414	-	-	0/12/33/33	0/1/3/3
3	NDG	D	479	1	-	0/6/23/26	0/1/1/1
6	HTQ	E	5[Y]	-	-	0/12/33/33	0/1/3/3
6	HTQ	E	5[Z]	-	-	0/12/33/33	0/1/3/3
6	HTQ	E	515	-	-	0/12/33/33	0/1/3/3
2	NAG	E	579	1	-	0/6/23/26	0/1/1/1
2	NAG	E	580	-	-	0/6/23/26	0/1/1/1
6	HTQ	F	6[Y]	-	-	0/12/33/33	0/1/3/3
6	HTQ	F	6[Z]	-	-	0/12/33/33	0/1/3/3
6	HTQ	F	616	-	-	0/12/33/33	0/1/3/3
3	NDG	F	679	1	-	1/6/23/26	0/1/1/1
4	SIA	F	682	-	-	0/14/38/38	0/1/1/1

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	111	HTQ	C2-C1	2.10	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1[Y]	HTQ	C13-C11	2.11	1.55	1.52
6	F	6[Z]	HTQ	C13-C11	2.12	1.55	1.52
6	A	1[Z]	HTQ	C14-C13	2.12	1.56	1.51
6	D	414	HTQ	C13-C11	2.13	1.55	1.52

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	182	SIA	C7-C6-C5	-2.83	110.03	114.32
2	A	179	NAG	C2-N2-C7	-2.41	119.94	123.04
2	E	579	NAG	C2-N2-C7	-2.29	120.10	123.04
3	B	279	NDG	C2-N2-C7	-2.21	120.20	123.04
2	E	580	NAG	C2-N2-C7	-2.19	120.22	123.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	679	NDG	O7-C7-N2-C2

There are no ring outliers.

26 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1[Y]	HTQ	4	0
6	A	1[Z]	HTQ	4	0
6	A	111	HTQ	13	0
4	A	182	SIA	5	0
6	B	2[Y]	HTQ	4	0
6	B	2[Z]	HTQ	1	0
6	B	212	HTQ	9	0
3	B	279	NDG	3	0
4	B	282	SIA	17	0
6	C	3[Y]	HTQ	4	0
6	C	3[Z]	HTQ	4	0
6	C	313	HTQ	3	0
6	D	4[Y]	HTQ	2	0
6	D	4[Z]	HTQ	3	0
6	D	414	HTQ	7	0
3	D	479	NDG	2	0
6	E	5[Y]	HTQ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	5[Z]	HTQ	1	0
6	E	515	HTQ	12	0
2	E	579	NAG	2	0
2	E	580	NAG	2	0
6	F	6[Y]	HTQ	3	0
6	F	6[Z]	HTQ	3	0
6	F	616	HTQ	7	0
3	F	679	NDG	3	0
4	F	682	SIA	5	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.