



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:05 am 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

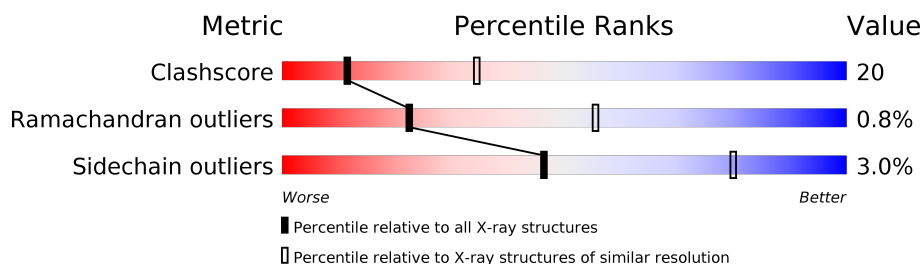
1 Overall quality at a glance

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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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 crite-

ria:

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:

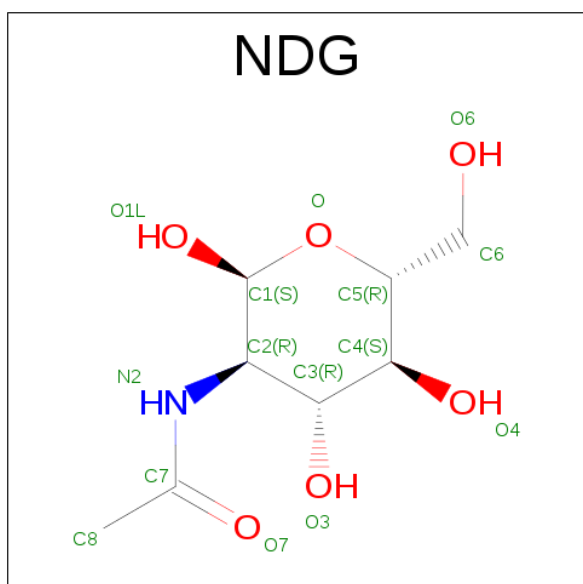
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141
D	?	-	GLN	DELETION	UNP P23141
E	?	-	GLN	DELETION	UNP P23141
F	?	-	GLN	DELETION	UNP P23141

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



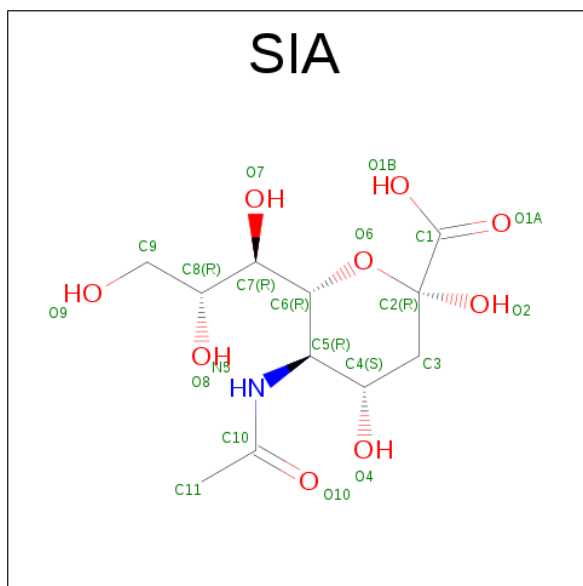
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

- 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: $C_{11}H_{19}NO_9$).

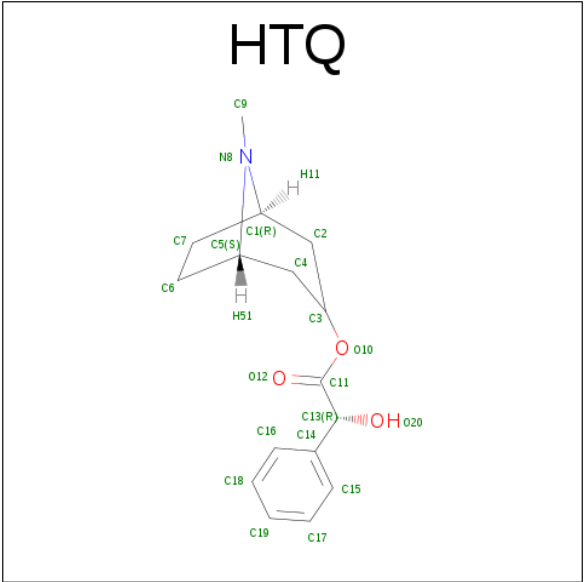


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	11	1	9		
4	B	1	Total	C	N	O	0	0
			21	11	1	9		
4	F	1	Total	C	N	O	0	0
			21	11	1	9		

- 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		
	B	1	Total	C	N	O		
			20	16	1	3		
	C	1	Total	C	N	O		
			20	16	1	3		
6	D	1	Total	C	N	O	0	0
			20	16	1	3		
	E	1	Total	C	N	O		
			20	16	1	3		
	F	1	Total	C	N	O		
			20	16	1	3		
6	A	1	Total	C	N	O	0	1
			40	32	2	6		
	B	1	Total	C	N	O		
			40	32	2	6		
	C	1	Total	C	N	O		
			40	32	2	6		
6	D	1	Total	C	N	O	0	1
			40	32	2	6		
	E	1	Total	C	N	O		
			40	32	2	6		
	F	1	Total	C	N	O		
			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

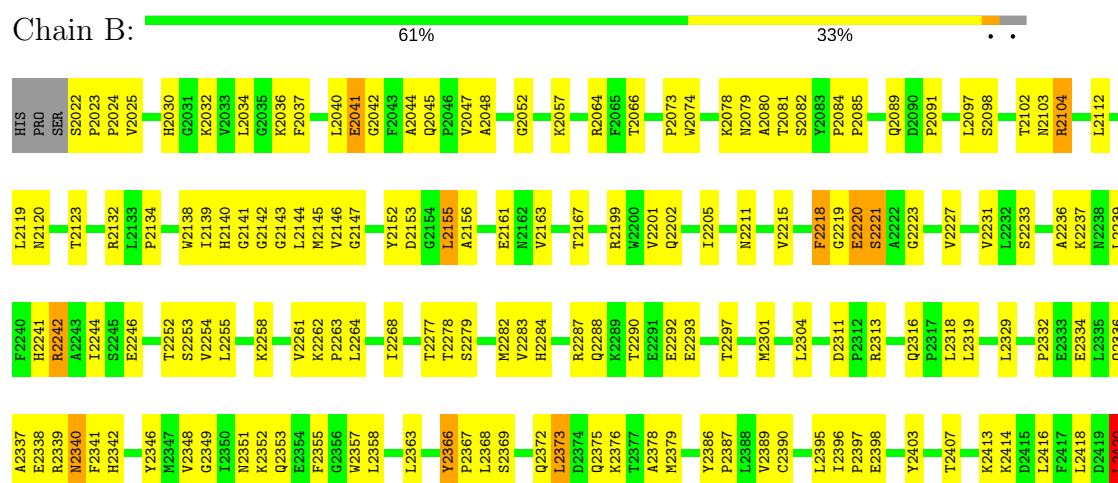
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

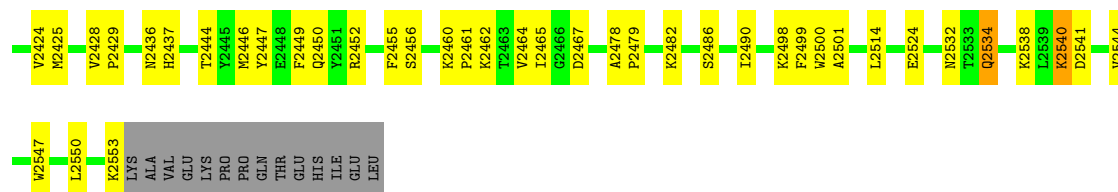
Note EDS was not executed.

• Molecule 1: liver Carboxylesterase I



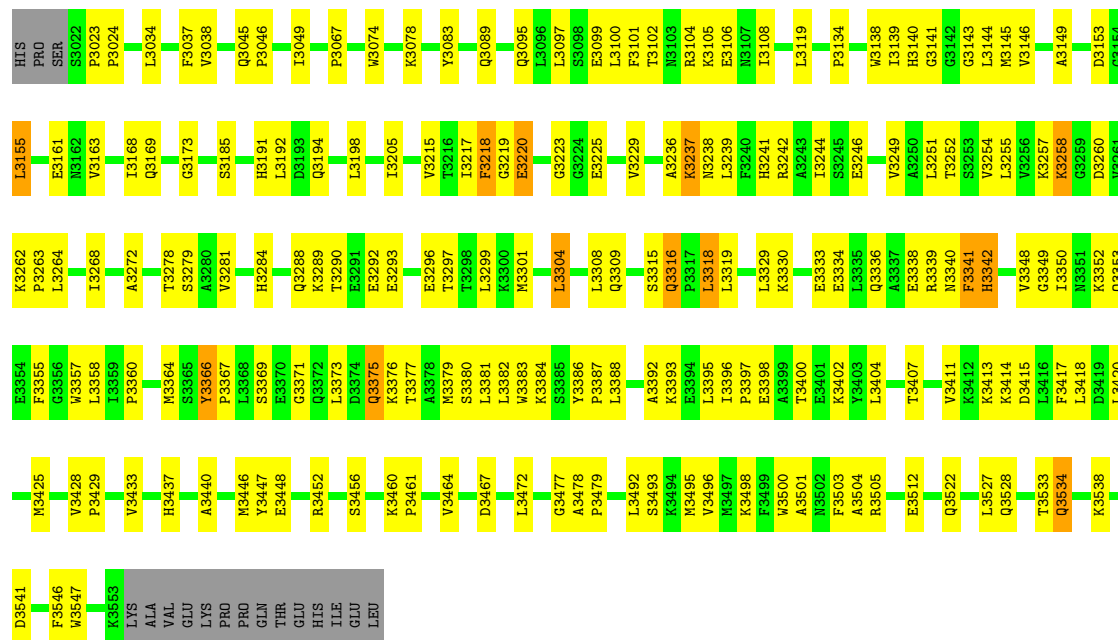
• Molecule 1: liver Carboxylesterase I





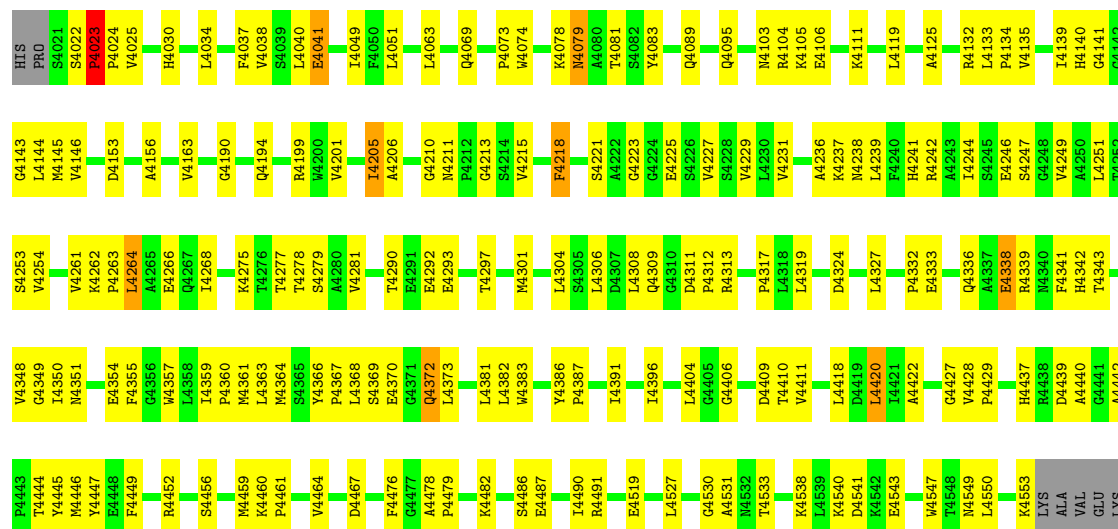
• Molecule 1: liver Carboxylesterase I

Chain C: 62% 32% ..



• Molecule 1: liver Carboxylesterase I

Chain D: 64% 32% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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

Continued on next page...

Continued from previous page...

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%)	38	72
1	B	529/548 (96%)	496 (94%)	28 (5%)	5 (1%)	20	52
1	C	529/548 (96%)	488 (92%)	38 (7%)	3 (1%)	28	62
1	D	530/548 (97%)	503 (95%)	23 (4%)	4 (1%)	22	55
1	E	529/548 (96%)	495 (94%)	27 (5%)	7 (1%)	14	41
1	F	529/548 (96%)	493 (93%)	32 (6%)	4 (1%)	22	55
All	All	3176/3288 (97%)	2970 (94%)	181 (6%)	25 (1%)	22	55

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%)	53	84
1	B	447/463 (96%)	433 (97%)	14 (3%)	45	79
1	C	447/463 (96%)	432 (97%)	15 (3%)	42	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	448/463 (97%)	437 (98%)	11 (2%)	53	84
1	E	447/463 (96%)	431 (96%)	16 (4%)	40	74
1	F	447/463 (96%)	433 (97%)	14 (3%)	45	79
All	All	2684/2778 (97%)	2603 (97%)	81 (3%)	46	80

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	9 (40%)	30,31,31	1.50	3 (10%)
6	HTQ	A	1[Z]	-	22,22,22	2.13	9 (40%)	30,31,31	1.80	3 (10%)
6	HTQ	A	111	-	22,22,22	1.94	8 (36%)	30,31,31	1.76	5 (16%)
2	NAG	A	179	1	14,14,15	0.61	0	15,19,21	0.73	1 (6%)
4	SIA	A	182	-	18,21,21	1.07	2 (11%)	19,31,31	0.94	1 (5%)
6	HTQ	B	2[Y]	-	22,22,22	2.00	8 (36%)	30,31,31	1.21	2 (6%)
6	HTQ	B	2[Z]	-	22,22,22	2.03	8 (36%)	30,31,31	1.38	3 (10%)
6	HTQ	B	212	-	22,22,22	1.90	7 (31%)	30,31,31	1.67	4 (13%)
3	NDG	B	279	1	14,14,15	0.51	0	15,19,21	0.82	0
4	SIA	B	282	-	18,21,21	1.27	2 (11%)	19,31,31	1.11	1 (5%)
6	HTQ	C	3[Y]	-	22,22,22	2.05	8 (36%)	30,31,31	1.53	5 (16%)
6	HTQ	C	3[Z]	-	22,22,22	2.10	8 (36%)	30,31,31	1.47	5 (16%)
6	HTQ	C	313	-	22,22,22	2.04	8 (36%)	30,31,31	1.44	2 (6%)
2	NAG	C	379	1	14,14,15	0.55	0	15,19,21	0.69	0
6	HTQ	D	4[Y]	-	22,22,22	2.03	8 (36%)	30,31,31	1.42	4 (13%)
6	HTQ	D	4[Z]	-	22,22,22	1.97	8 (36%)	30,31,31	1.26	2 (6%)
6	HTQ	D	414	-	22,22,22	2.06	8 (36%)	30,31,31	2.02	4 (13%)
3	NDG	D	479	1	14,14,15	0.52	0	15,19,21	0.68	0
6	HTQ	E	5[Y]	-	22,22,22	2.05	8 (36%)	30,31,31	1.32	4 (13%)
6	HTQ	E	5[Z]	-	22,22,22	2.06	9 (40%)	30,31,31	1.49	2 (6%)
6	HTQ	E	515	-	22,22,22	2.02	8 (36%)	30,31,31	1.47	2 (6%)
2	NAG	E	579	1	14,14,15	0.55	0	15,19,21	0.70	0
2	NAG	E	580	-	14,14,15	0.53	0	15,19,21	0.67	0
6	HTQ	F	6[Y]	-	22,22,22	2.08	8 (36%)	30,31,31	1.39	2 (6%)
6	HTQ	F	6[Z]	-	22,22,22	2.08	9 (40%)	30,31,31	1.51	3 (10%)
6	HTQ	F	616	-	22,22,22	1.91	9 (40%)	30,31,31	1.39	2 (6%)
3	NDG	F	679	1	14,14,15	0.60	0	15,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SIA	F	682	-	18,21,21	1.26	2 (11%)	19,31,31	0.73	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 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	111	HTQ	C2-C1	2.01	1.57	1.53
6	F	616	HTQ	C17-C15	2.01	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1[Y]	HTQ	C13-C11	2.12	1.55	1.52
4	F	682	SIA	O6-C2	2.13	1.45	1.43
6	F	6[Z]	HTQ	C13-C11	2.13	1.55	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	111	HTQ	C2-C1-N8	-2.14	104.71	107.64
6	C	3[Z]	HTQ	C2-C1-N8	-2.07	104.80	107.64
2	A	179	NAG	C2-N2-C7	-2.06	119.94	122.94
6	C	3[Y]	HTQ	C2-C1-N8	-2.06	104.82	107.64
6	B	212	HTQ	O10-C11-O12	2.06	127.93	123.90

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
6	E	5[Z]	HTQ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.