



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:38 AM GMT

PDB ID : 2DQY
Title : Crystal structure of human carboxylesterase in complex with cholate and palmitate
Authors : Bencharit, S.; Edwards, C.C.; Morton, C.L.; Howard-Williams, E.L.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2006-06-02
Resolution : 3.00 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

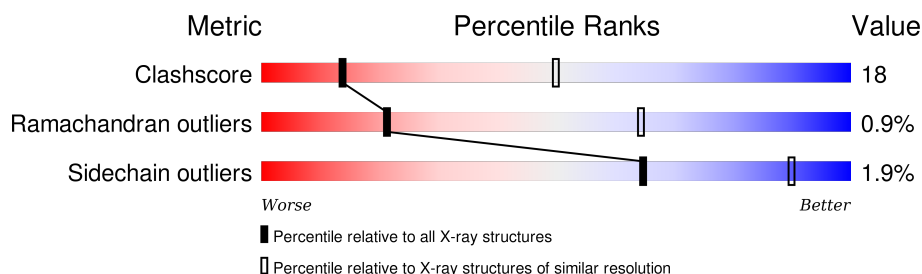
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	542	
1	B	542	
1	C	542	

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	C	379	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PLM	A	11	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12967 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.

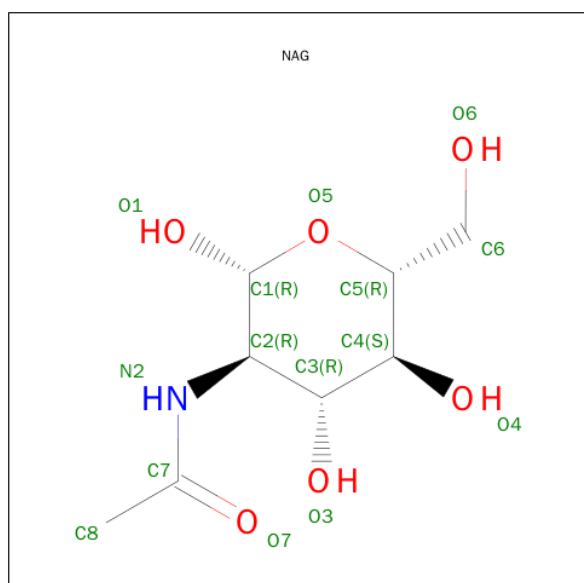
- Molecule 1 is a protein called Liver carboxylesterase 1.

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	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			

There are 3 discrepancies between the modelled and reference sequences:

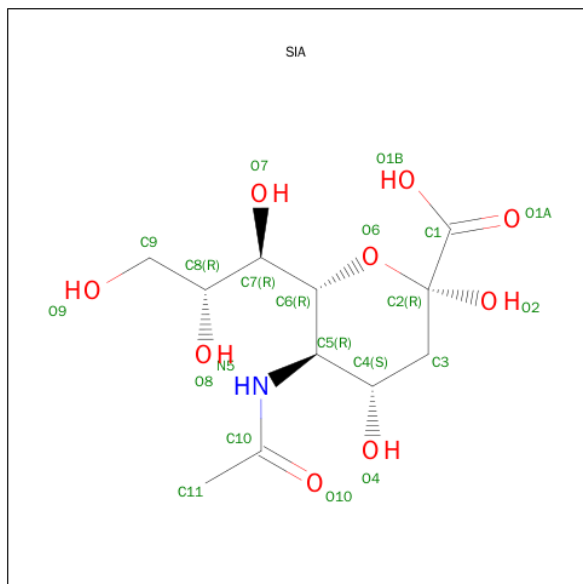
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141

- 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	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		

- Molecule 3 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



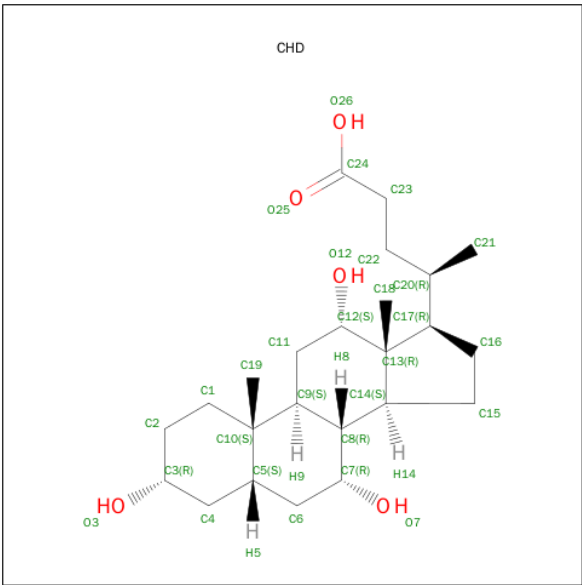
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



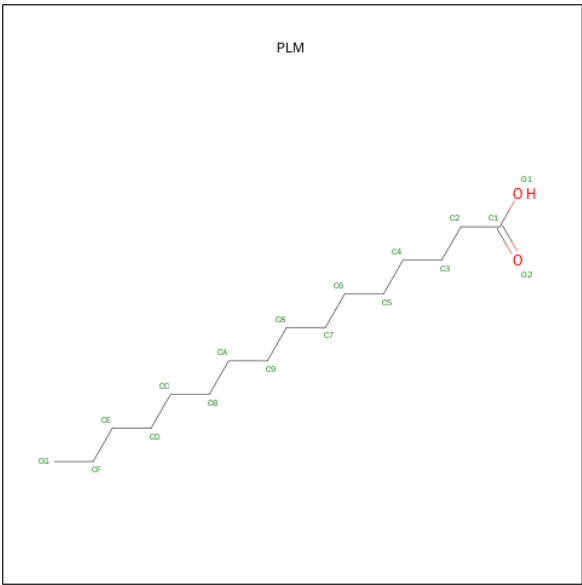
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			29	24	5		
5	B	1	Total	C	O	0	0
			29	24	5		
5	C	1	Total	C	O	0	0
			29	24	5		

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			18	16	2		
6	C	1	Total	C	O	0	0
			18	16	2		

- Molecule 7 is water.

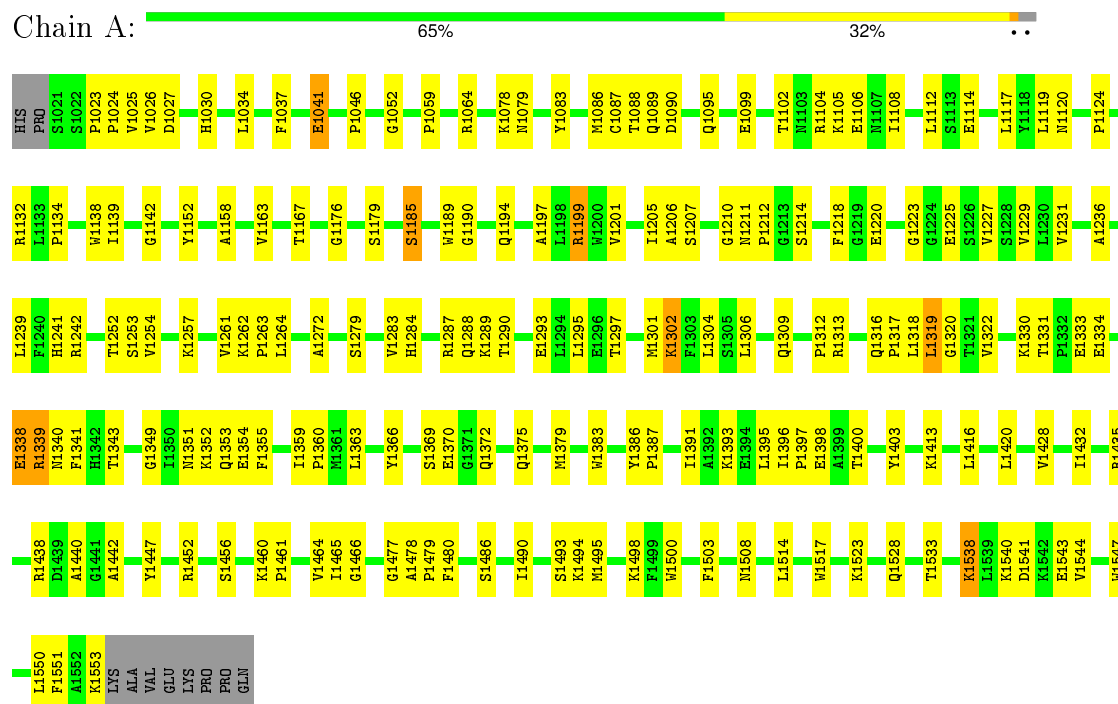
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total	O	0	0
			108	108		
7	B	87	Total	O	0	0
			87	87		
7	C	106	Total	O	0	0
			106	106		

3 Residue-property plots

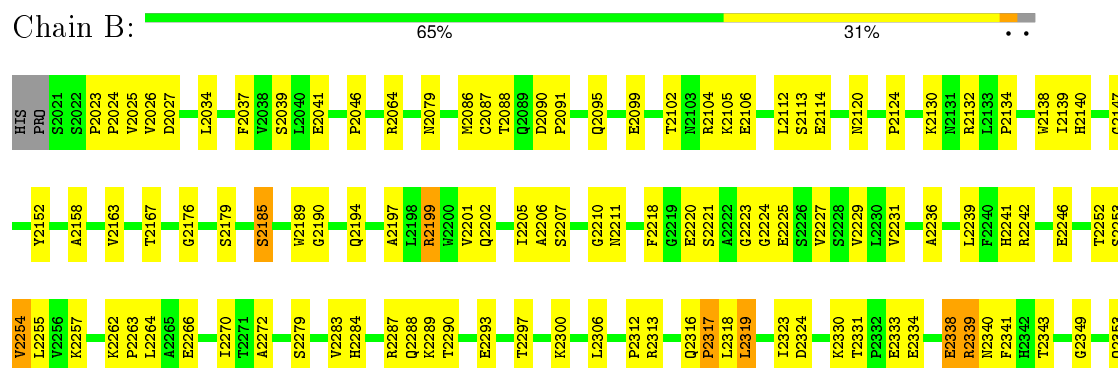
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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 1



- Molecule 1: Liver carboxylesterase 1



PRO	GLN	R2452	S2456	L2358	K2460	P2461	V2464	L2465	G2466	D2467	H2468	G2477	A2478	P2479	E2487	S2493	K2494	M2495	K2498	P2499	W2500	F2503	L2514	W2517	K2523	Q2528	N2532	T2533	K2538	K2540	D2541	K2542	E2543	V2544	W2547	L2550	F2551	A2552	K2553	LYS	ALA	VAL	GLU	LYS	PRO	P2355	L2359	P2360	H2361	L2363	M2364	S2366	P2367	L2368	S2369	E2370	G2371	Q2372	M2379	W2383	K2384	S2385	Y2386	P2387	L2388	V2389	C2390	K2393	E2394	L2395	L2396	P2397	T2400	Y2403	L2404	K2413	L2416	L2420	V2428	L2432	R2435	R2438	D2439	A2440	G2441	A2442	Y2447
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• Molecule 1: Liver carboxylesterase 1



K3553	LYS	ALA	VAL	GLU	LYS	PRO	GLN	G3441	A3442	Y3447	R3452	P3461	K3463	T3463	V3464	D3467	G3477	A3478	P3479	F3480	S3486	T3490	S3493	K3494	M3495	K3498	F3499	W3500	F3503	A3504	R3505	M3506	G3507	G3513	L3514	W3517	K3523	Q3528	T3533	K3538	L3539	K3540	D3541	K3542	E3543	V3544	W3547	L3550	D3439	A3440	L3264	A3265	E3266	Q3267	L3268	A3269	I3270	T3271	A3272	K3275	T3276	T3277	T3278	S3279	V3283	L3284	K3287	Q3288	K3289	T3290	E3293	L3294	L3295	T3297	K3300	M3301	K3302	F3303	L3304	S3305	L3306	P3312	R3313	Q3316	P3317	L3318	T3323	L3329	K3330	T3331	F3332	E3333	E3334	E3338	R3339	M3340	T3343	T3167	G3176	S3179	S3185	K3189	G3190	Q3194	V3195	A3196	A3197	L3198	R3199	K3200	V3201	A3206	G3210	M3211	F3218	G3219	E3220	G3223	G3224	E3225	S3226	V3227	S3228	V3229	L3230	V3231	A3236	L3239	F3240	R3241	R3242	P3124	R3132	L3133	P3134	W3138	S3253	T3139	Y3152	A3158	V3163	HIS	PRO	S3021	P3023	P3024	V3025	D3027	L3034	F3037	E3041	Q3045	P3058	P3059	L3063	P3068	M3079	M3086	C3087	T3088	T3102	M3103	R3104	K3105	E3106	P3109	L3112	L3117	Y3118	L3119	M3120	P3124	R3132	L3133	P3134	W3138	S3253	T3139	Y3152	A3158	V3163
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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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.29 Å 179.88 Å 201.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 3.00	Depositor
% Data completeness (in resolution range)	93.0 (19.93-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12967	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: PLM, SIA, CHD, NAG, SO4

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	0.43	0/4236	0.60	1/5754 (0.0%)
1	B	0.42	0/4236	0.58	0/5754
1	C	0.42	0/4236	0.58	0/5754
All	All	0.42	0/12708	0.59	1/17262 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1319	LEU	N-CA-C	-7.63	90.40	111.00

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	165	0
1	B	4130	0	4131	143	0
1	C	4130	0	4131	153	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	2	0
3	A	21	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	18	2	0
3	C	21	0	18	8	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
5	A	29	0	39	2	0
5	B	29	0	39	0	0
5	C	29	0	39	7	0
6	A	18	0	31	9	0
6	B	18	0	31	2	0
6	C	18	0	31	7	0
7	A	108	0	0	14	0
7	B	87	0	0	11	0
7	C	106	0	0	22	0
All	All	12967	0	12696	468	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 18.

The worst 5 of 468 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2317:PRO:HG3	1:B:2387:PRO:HB2	1.29	1.06
1:A:1199:ARG:HH11	1:A:1199:ARG:HB3	1.28	0.97
1:C:3199:ARG:HB3	1:C:3199:ARG:HH11	1.31	0.95
1:B:2199:ARG:HB3	1:B:2199:ARG:HH11	1.26	0.95
1:B:2105:LYS:HE2	1:B:2106:GLU:HG2	1.51	0.93

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	530/542 (98%)	481 (91%)	45 (8%)	4 (1%)	24	66
1	B	530/542 (98%)	478 (90%)	44 (8%)	8 (2%)	13	50
1	C	530/542 (98%)	484 (91%)	43 (8%)	3 (1%)	30	72
All	All	1590/1626 (98%)	1443 (91%)	132 (8%)	15 (1%)	21	64

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1185	SER
1	B	2185	SER
1	B	2319	LEU
1	B	2369	SER
1	C	3185	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	448/457 (98%)	440 (98%)	8 (2%)	66	91
1	B	448/457 (98%)	439 (98%)	9 (2%)	63	89
1	C	448/457 (98%)	439 (98%)	9 (2%)	63	89
All	All	1344/1371 (98%)	1318 (98%)	26 (2%)	65	90

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2264	LEU
1	B	2366	TYR
1	C	3500	TRP
1	B	2338	GLU
1	B	2339	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2131	ASN
1	B	2316	GLN
1	C	3372	GLN
1	B	2238	ASN
1	B	2372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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
5	CHD	A	1	-	29,32,32	2.03	13 (44%)	48,51,51	1.31	6 (12%)
6	PLM	A	11	-	14,17,17	0.38	0	14,17,17	0.43	0
2	NAG	A	179	1	14,14,15	0.80	0	15,19,21	1.16	2 (13%)
3	SIA	A	182	-	17,21,21	1.05	2 (11%)	19,31,31	1.04	2 (10%)
4	SO4	A	184	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	A	185	-	4,4,4	0.35	0	6,6,6	0.14	0
4	SO4	A	285	-	4,4,4	0.28	0	6,6,6	0.11	0
6	PLM	B	12	-	14,17,17	0.44	0	14,17,17	0.43	0
5	CHD	B	2	-	29,32,32	2.16	15 (51%)	48,51,51	1.33	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	279	1	14,14,15	0.53	0	15,19,21	1.13	1 (6%)
3	SIA	B	282	-	17,21,21	0.86	0	19,31,31	1.02	1 (5%)
4	SO4	B	284	-	4,4,4	0.20	0	6,6,6	0.16	0
6	PLM	C	13	-	14,17,17	0.42	0	14,17,17	0.43	0
5	CHD	C	3	-	29,32,32	2.06	11 (37%)	48,51,51	1.31	7 (14%)
2	NAG	C	379	1	14,14,15	0.63	0	15,19,21	1.13	2 (13%)
3	SIA	C	382	-	17,21,21	1.06	2 (11%)	19,31,31	1.19	2 (10%)
4	SO4	C	384	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	C	385	-	4,4,4	0.29	0	6,6,6	0.12	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
5	CHD	A	1	-	-	0/7/74/74	0/4/4/4
6	PLM	A	11	-	-	0/13/15/15	0/0/0/0
2	NAG	A	179	1	-	0/6/23/26	0/1/1/1
3	SIA	A	182	-	-	0/14/38/38	0/1/1/1
4	SO4	A	184	-	-	0/0/0/0	0/0/0/0
4	SO4	A	185	-	-	0/0/0/0	0/0/0/0
4	SO4	A	285	-	-	0/0/0/0	0/0/0/0
6	PLM	B	12	-	-	0/13/15/15	0/0/0/0
5	CHD	B	2	-	-	0/7/74/74	0/4/4/4
2	NAG	B	279	1	-	0/6/23/26	0/1/1/1
3	SIA	B	282	-	-	1/14/38/38	0/1/1/1
4	SO4	B	284	-	-	0/0/0/0	0/0/0/0
6	PLM	C	13	-	-	0/13/15/15	0/0/0/0
5	CHD	C	3	-	-	0/7/74/74	0/4/4/4
2	NAG	C	379	1	1/1/5/7	0/6/23/26	0/1/1/1
3	SIA	C	382	-	-	0/14/38/38	0/1/1/1
4	SO4	C	384	-	-	0/0/0/0	0/0/0/0
4	SO4	C	385	-	-	0/0/0/0	0/0/0/0

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	CHD	C4-C3	2.05	1.55	1.51
5	A	1	CHD	C4-C3	2.09	1.55	1.51
5	B	2	CHD	C1-C2	2.16	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	CHD	C6-C7	2.19	1.56	1.52
3	C	382	SIA	C7-C6	2.19	1.55	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2	CHD	C17-C13-C14	-4.11	95.90	100.05
2	B	279	NAG	C2-N2-C7	-3.98	117.92	123.04
5	C	3	CHD	C19-C10-C1	-3.59	102.16	108.20
5	A	1	CHD	C9-C11-C12	-3.38	110.09	114.36
5	A	1	CHD	C17-C13-C14	-3.23	96.79	100.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	379	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	282	SIA	O10-C10-N5-C5

There are no ring outliers.

9 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	CHD	2	0
6	A	11	PLM	9	0
3	A	182	SIA	3	0
6	B	12	PLM	2	0
3	B	282	SIA	2	0
6	C	13	PLM	7	0
5	C	3	CHD	7	0
2	C	379	NAG	2	0
3	C	382	SIA	8	0

5.7 Other polymers [i](#)

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](#)

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.