



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2H7C  
Title : Crystal structure of human carboxylesterase in complex with Coenzyme A  
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 : 2.00 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](mailto: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.

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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

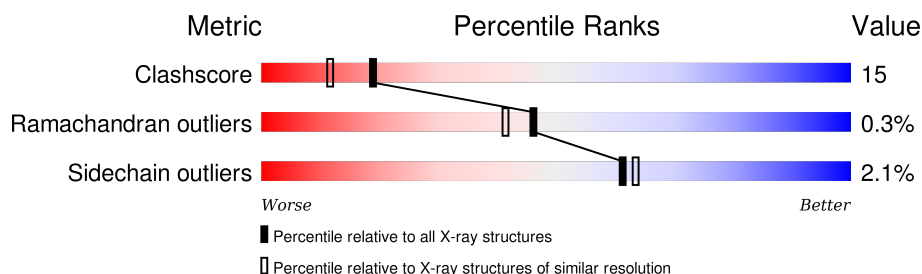
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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  $\geq 3$ , 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	
1	D	542	
1	E	542	
1	F	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
5	SIA	D	482	-	-	X	-
7	COA	A	1	X	-	X	-
7	COA	B	2	X	-	X	-
7	COA	C	3	X	-	X	-
7	COA	D	4	X	-	X	-
7	COA	E	5	X	-	X	-
7	COA	F	6	X	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27978 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	1	0
			4132	2663	686	762	21			
1	B	531	Total	C	N	O	S	0	1	0
			4104	2646	681	756	21			
1	C	531	Total	C	N	O	S	0	1	0
			4130	2662	685	762	21			
1	D	532	Total	C	N	O	S	0	1	0
			4136	2665	686	764	21			
1	E	531	Total	C	N	O	S	0	1	0
			4130	2662	685	762	21			
1	F	531	Total	C	N	O	S	0	1	0
			4129	2662	685	761	21			

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 a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

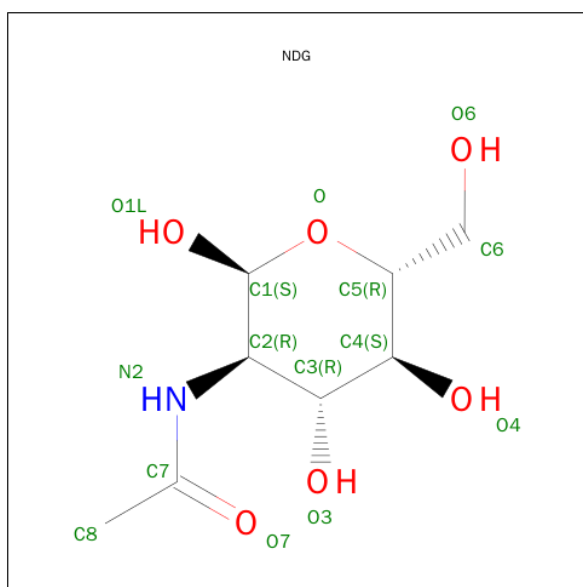
- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



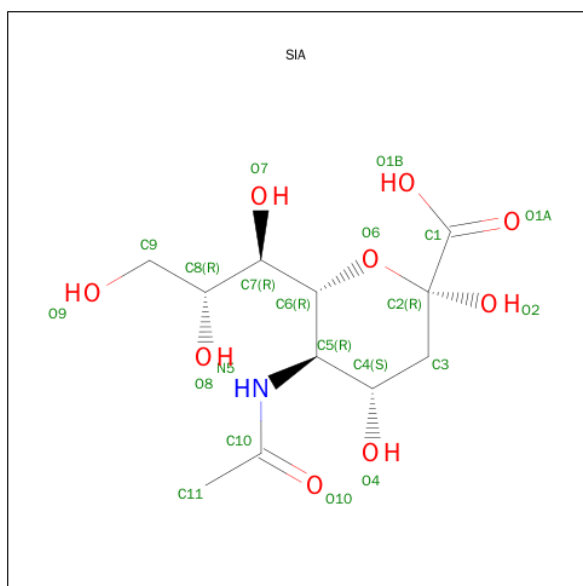
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



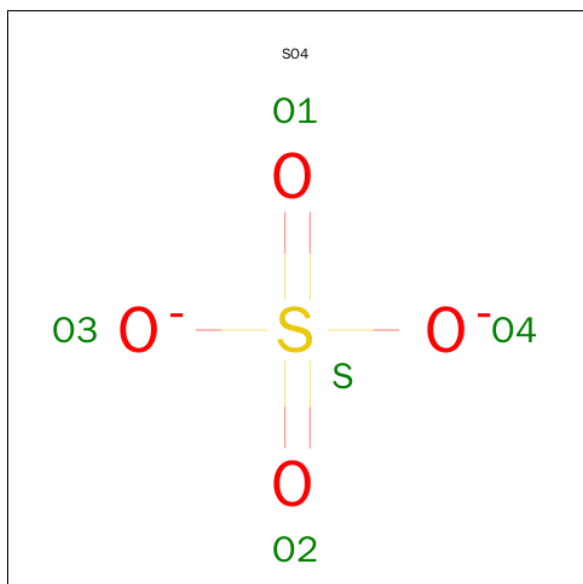
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



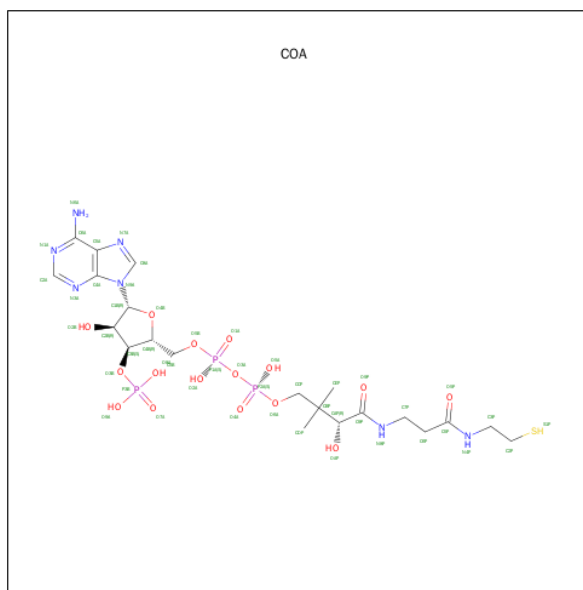
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			21	11	1	9		
5	E	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

- Molecule 7 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
7	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
7	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
7	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
7	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
7	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	474	Total 474	O 474	0	0
8	B	500	Total 500	O 500	0	0
8	C	404	Total 404	O 404	0	0
8	D	480	Total 480	O 480	0	0
8	E	448	Total 448	O 448	0	0
8	F	409	Total 409	O 409	0	0

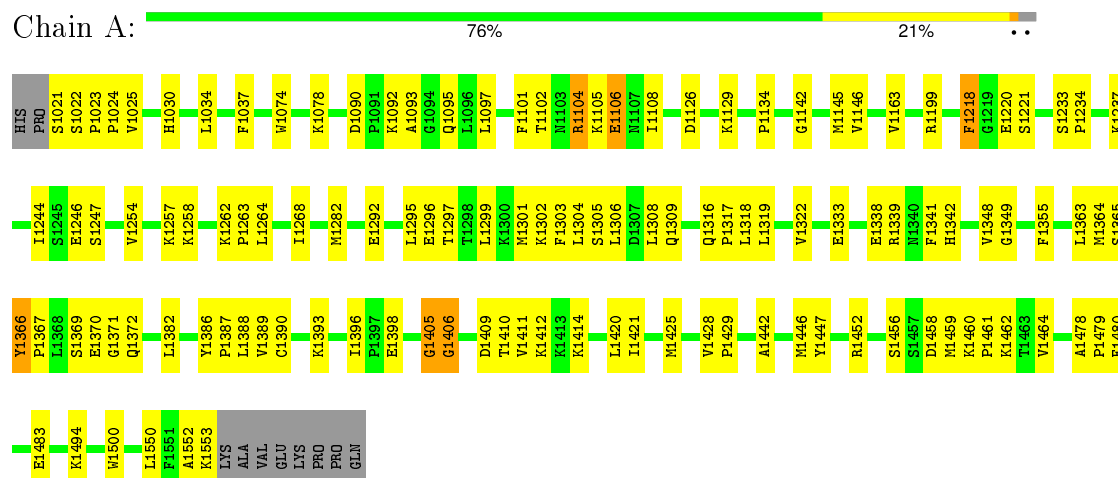


### 3 Residue-property plots

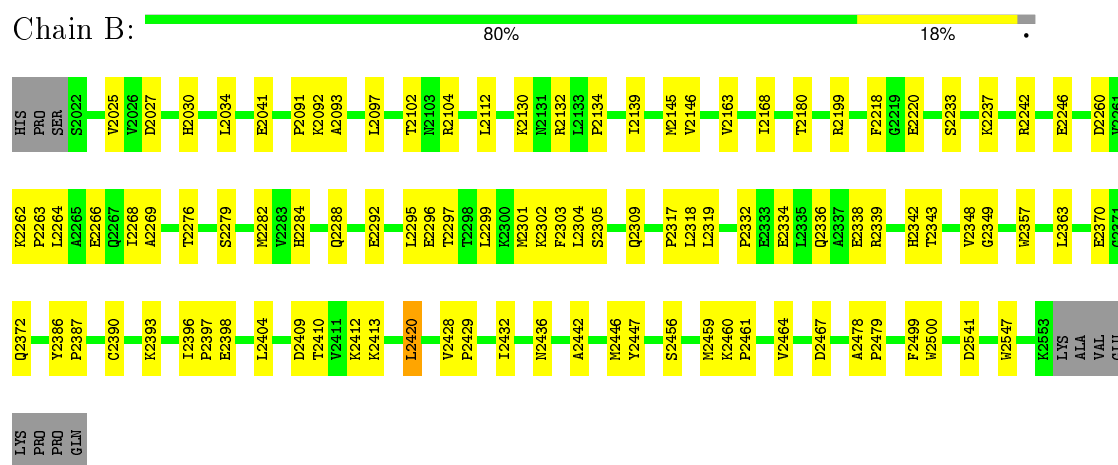
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



- Molecule 1: Liver carboxylesterase 1



- Molecule 1: Liver carboxylesterase 1

Chain D:  77% 20% 3%

- Molecule 1: Liver carboxylesterase 1

Chain E:  75% 22%

- Molecule 1: Liver carboxylesterase 1

Chain F:  76% 21% ..



## 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, $\alpha$ , $\beta$ , $\gamma$	88.99 Å   115.37 Å   175.53 Å 90.00°   90.05°   90.00°	Depositor
Resolution (Å)	29.10 – 2.00	Depositor
% Data completeness (in resolution range)	97.1 (29.10-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.183 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: COA, SIA, NAG, NDG, 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	0.33	0/4238	0.58	0/5757
1	B	0.33	0/4210	0.58	0/5725
1	C	0.31	0/4236	0.57	0/5754
1	D	0.33	0/4242	0.60	1/5762 (0.0%)
1	E	0.32	0/4236	0.56	0/5754
1	F	0.32	0/4236	0.56	0/5754
All	All	0.32	0/25398	0.58	1/34506 (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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4420	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	3390[B]	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	D	4390[B]	CYS	Mainchain

## 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	4132	0	4131	140	0
1	B	4104	0	4075	121	0
1	C	4130	0	4129	141	0
1	D	4136	0	4135	133	0
1	E	4130	0	4130	135	0
1	F	4129	0	4130	144	0
2	A	28	0	25	1	0
2	F	28	0	25	4	0
3	B	14	0	13	1	0
3	D	14	0	13	0	0
3	E	14	0	13	1	0
4	C	14	0	13	1	0
5	D	21	0	18	9	0
5	E	21	0	18	5	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	15	0	0	0	0
6	E	5	0	0	0	0
6	F	10	0	0	0	0
7	A	48	0	32	28	0
7	B	48	0	32	30	0
7	C	48	0	32	21	0
7	D	48	0	32	25	0
7	E	48	0	32	24	0
7	F	48	0	32	28	0
8	A	474	0	0	14	0
8	B	500	0	0	21	0
8	C	404	0	0	20	0
8	D	480	0	0	19	0
8	E	448	0	0	20	0
8	F	409	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27978	0	25060	770	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 15.

The worst 5 of 770 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:3258:LYS:H	1:C:3258:LYS:HD3	1.12	1.15
1:B:2093:ALA:HB1	7:B:2:COA:H121	1.35	1.08
2:F:679:NAG:H61	2:F:680:NAG:H83	1.33	1.08
1:A:1093:ALA:HB1	7:A:1:COA:H121	1.42	1.00
1:C:3414:LYS:HZ3	1:E:5370:GLU:HA	1.25	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	531/542 (98%)	505 (95%)	24 (4%)	2 (0%)	39	33
1	B	530/542 (98%)	512 (97%)	17 (3%)	1 (0%)	52	48
1	C	530/542 (98%)	506 (96%)	22 (4%)	2 (0%)	39	33
1	D	531/542 (98%)	509 (96%)	20 (4%)	2 (0%)	39	33
1	E	530/542 (98%)	509 (96%)	20 (4%)	1 (0%)	52	48
1	F	530/542 (98%)	511 (96%)	17 (3%)	2 (0%)	39	33
All	All	3182/3252 (98%)	3052 (96%)	120 (4%)	10 (0%)	46	41

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1406	GLY
1	C	3410	THR
1	D	4410	THR
1	E	5341	PHE
1	F	6405	GLY

### 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%)	441 (98%)	7 (2%)	70	73
1	B	440/457 (96%)	433 (98%)	7 (2%)	70	73
1	C	448/457 (98%)	433 (97%)	15 (3%)	45	43
1	D	449/457 (98%)	438 (98%)	11 (2%)	57	58
1	E	448/457 (98%)	441 (98%)	7 (2%)	70	73
1	F	448/457 (98%)	439 (98%)	9 (2%)	63	65
All	All	2681/2742 (98%)	2625 (98%)	56 (2%)	61	63

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3420	LEU
1	D	4264	LEU
1	F	6414	LYS
1	C	3500	TRP
1	C	3534	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4030	HIS
1	D	4340	ASN
1	F	6506	ASN
1	D	4107	ASN

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Mol	Chain	Res	Type
1	D	4353	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 ⓘ

4 carbohydrates 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	NAG	A	179	1,2	14,14,15	0.65	0	15,19,21	0.92	1 (6%)
2	NAG	A	180	2	14,14,15	0.83	0	15,19,21	1.22	2 (13%)
2	NAG	F	679	1,2	14,14,15	0.54	0	15,19,21	0.72	1 (6%)
2	NAG	F	680	2	14,14,15	0.55	0	15,19,21	0.66	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
2	NAG	A	179	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	180	2	-	1/6/23/26	0/1/1/1
2	NAG	F	679	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	680	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	180	NAG	C2-N2-C7	-2.54	119.78	123.04
2	F	679	NAG	C2-N2-C7	-2.24	120.16	123.04
2	A	179	NAG	C2-N2-C7	-2.23	120.17	123.04
2	A	180	NAG	C1-O5-C5	3.25	116.37	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	180	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	179	NAG	1	0
2	A	180	NAG	1	0
2	F	679	NAG	3	0
2	F	680	NAG	3	0

## 5.6 Ligand geometry [i](#)

24 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
7	COA	A	1	-	40,50,50	3.10	7 (17%)	50,75,75	3.05	17 (34%)
6	SO4	A	185	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	285	-	4,4,4	0.19	0	6,6,6	0.10	0
7	COA	B	2	-	40,50,50	3.04	7 (17%)	50,75,75	2.97	17 (34%)
3	NAG	B	279	1	14,14,15	0.51	0	15,19,21	0.84	1 (6%)
6	SO4	B	284	-	4,4,4	0.20	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	384	-	4,4,4	0.19	0	6,6,6	0.10	0
6	SO4	C	184	-	4,4,4	0.18	0	6,6,6	0.12	0
7	COA	C	3	-	40,50,50	3.09	7 (17%)	50,75,75	2.97	17 (34%)
4	NDG	C	379	1	14,14,15	0.56	0	15,19,21	0.77	1 (6%)
6	SO4	C	385	-	4,4,4	0.23	0	6,6,6	0.07	0
7	COA	D	4	-	40,50,50	3.03	7 (17%)	50,75,75	2.91	15 (30%)
3	NAG	D	479	1	14,14,15	0.47	0	15,19,21	0.80	1 (6%)
5	SIA	D	482	-	17,21,21	0.77	0	19,31,31	0.97	2 (10%)
6	SO4	D	484	-	4,4,4	0.21	0	6,6,6	0.09	0
6	SO4	D	485	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	D	684	-	4,4,4	0.19	0	6,6,6	0.13	0
7	COA	E	5	-	40,50,50	3.08	7 (17%)	50,75,75	2.98	16 (32%)
3	NAG	E	579	1	14,14,15	0.56	0	15,19,21	0.67	0
5	SIA	E	582	-	17,21,21	0.84	0	19,31,31	0.89	1 (5%)
6	SO4	E	585	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	F	584	-	4,4,4	0.21	0	6,6,6	0.12	0
7	COA	F	6	-	40,50,50	3.07	7 (17%)	50,75,75	2.98	17 (34%)
6	SO4	F	685	-	4,4,4	0.24	0	6,6,6	0.11	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
7	COA	A	1	-	1/1/11/13	0/44/64/64	0/3/3/3
6	SO4	A	185	-	-	0/0/0/0	0/0/0/0
6	SO4	A	285	-	-	0/0/0/0	0/0/0/0
7	COA	B	2	-	1/1/11/13	0/44/64/64	0/3/3/3
3	NAG	B	279	1	-	0/6/23/26	0/1/1/1
6	SO4	B	284	-	-	0/0/0/0	0/0/0/0
6	SO4	B	384	-	-	0/0/0/0	0/0/0/0
6	SO4	C	184	-	-	0/0/0/0	0/0/0/0
7	COA	C	3	-	1/1/11/13	0/44/64/64	0/3/3/3
4	NDG	C	379	1	-	0/6/23/26	0/1/1/1
6	SO4	C	385	-	-	0/0/0/0	0/0/0/0
7	COA	D	4	-	1/1/11/13	0/44/64/64	0/3/3/3
3	NAG	D	479	1	-	0/6/23/26	0/1/1/1
5	SIA	D	482	-	-	0/14/38/38	0/1/1/1
6	SO4	D	484	-	-	0/0/0/0	0/0/0/0
6	SO4	D	485	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	D	684	-	-	0/0/0/0	0/0/0/0
7	COA	E	5	-	1/1/11/13	0/44/64/64	0/3/3/3
3	NAG	E	579	1	-	0/6/23/26	0/1/1/1
5	SIA	E	582	-	-	0/14/38/38	0/1/1/1
6	SO4	E	585	-	-	0/0/0/0	0/0/0/0
6	SO4	F	584	-	-	0/0/0/0	0/0/0/0
7	COA	F	6	-	1/1/11/13	0/44/64/64	0/3/3/3
6	SO4	F	685	-	-	0/0/0/0	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2	COA	P2A-O4A	2.50	1.60	1.51
7	A	1	COA	P2A-O4A	2.50	1.60	1.51
7	D	4	COA	P2A-O4A	2.51	1.60	1.51
7	E	5	COA	P2A-O4A	2.52	1.60	1.51
7	F	6	COA	P2A-O4A	2.53	1.60	1.51

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2	COA	O9P-C9P-N8P	-10.70	101.62	123.08
7	C	3	COA	O9P-C9P-N8P	-10.49	102.03	123.08
7	A	1	COA	O9P-C9P-N8P	-10.47	102.08	123.08
7	E	5	COA	O9P-C9P-N8P	-10.46	102.10	123.08
7	F	6	COA	O9P-C9P-N8P	-10.40	102.22	123.08

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	4	COA	CAP
7	A	1	COA	CAP
7	F	6	COA	CAP
7	B	2	COA	CAP
7	C	3	COA	CAP

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 173 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1	COA	28	0
7	B	2	COA	30	0
3	B	279	NAG	1	0
7	C	3	COA	21	0
4	C	379	NDG	1	0
7	D	4	COA	25	0
5	D	482	SIA	9	0
7	E	5	COA	24	0
3	E	579	NAG	1	0
5	E	582	SIA	5	0
7	F	6	COA	28	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.