wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:39 AM GMT

PDB ID	:	2DR0
Title	:	Crystal structure of human carboxylesterase in complex with taurocholate
Authors	:	Bencharit, S.; Redinbo, M.R.
Deposited on	:	2006-06-02
Resolution	:	3.20 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 (i) symbol.

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

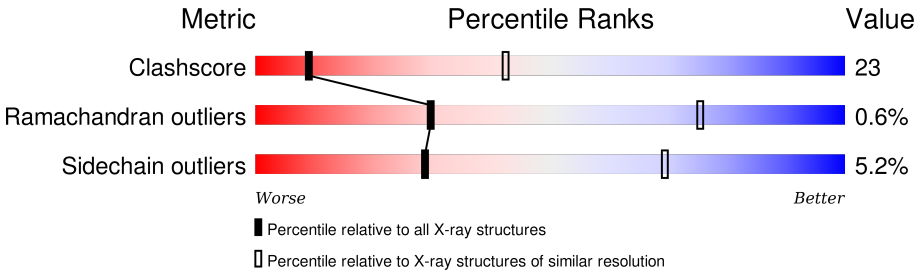
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 <=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	65% 30%
1	B	542	63% 32%
1	C	542	66% 30%

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
6	TCH	A	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TCH	A	102	X	-	X	-
6	TCH	B	201	X	-	-	-
6	TCH	B	202	X	-	X	-
6	TCH	C	301	X	-	-	-
6	TCH	C	302	X	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12988 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.

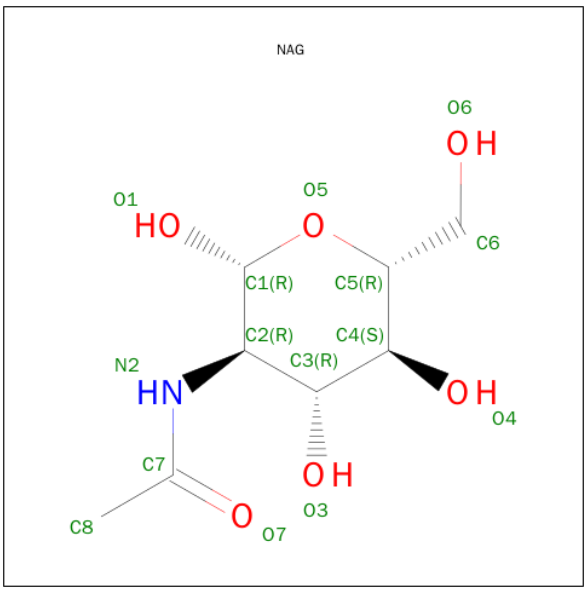
- Molecule 1 is a protein called Liver carboxylesterase 1.

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:

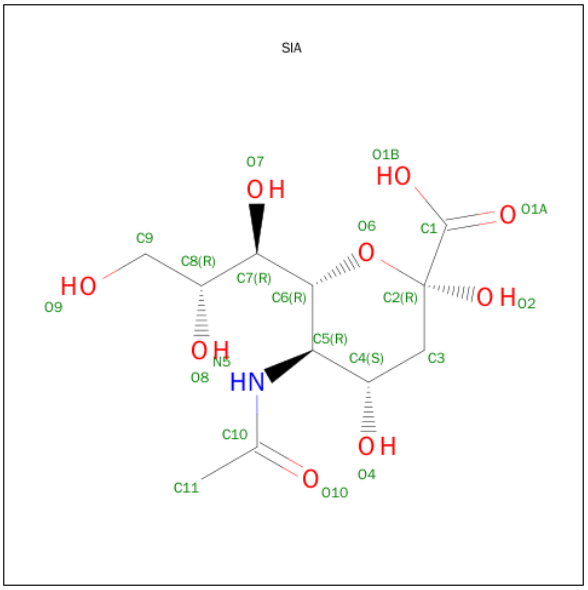
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141

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



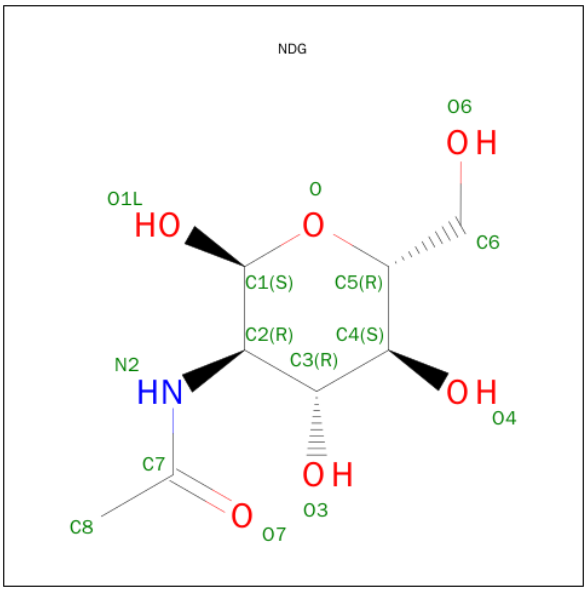
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

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



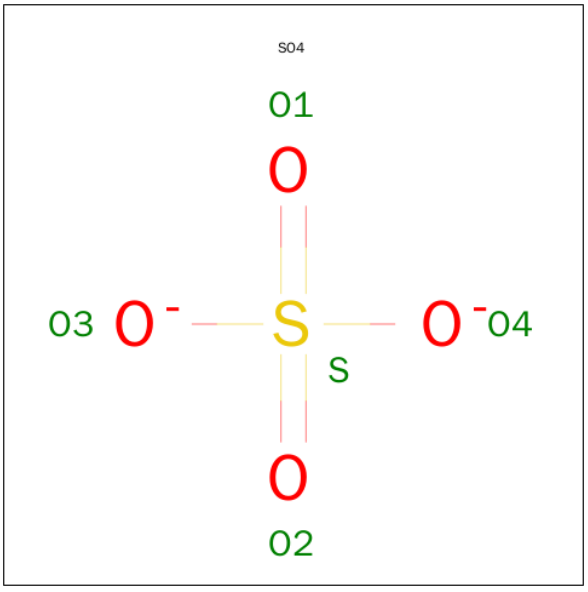
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 21 11 1 9	0	0
3	B	1	Total C N O 21 11 1 9	0	0
3	C	1	Total C N O 21 11 1 9	0	0

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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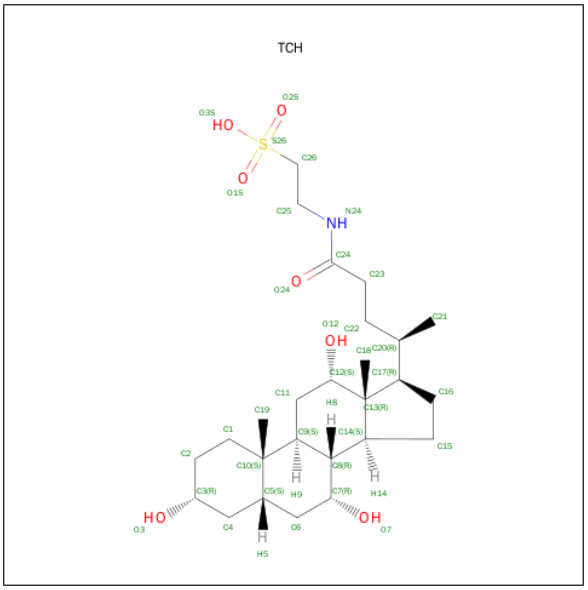
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is TAUROCHOLIC ACID (three-letter code: TCH) (formula: $C_{26}H_{45}NO_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 35 26 1 7 1	0	0
6	A	1	Total C N O S 35 26 1 7 1	0	0
6	B	1	Total C N O S 35 26 1 7 1	0	0
6	B	1	Total C N O S 35 26 1 7 1	0	0
6	C	1	Total C N O S 35 26 1 7 1	0	0
6	C	1	Total C N O S 35 26 1 7 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	104	Total O 104 104	0	0
7	B	72	Total O 72 72	0	0
7	C	77	Total O 77 77	0	0

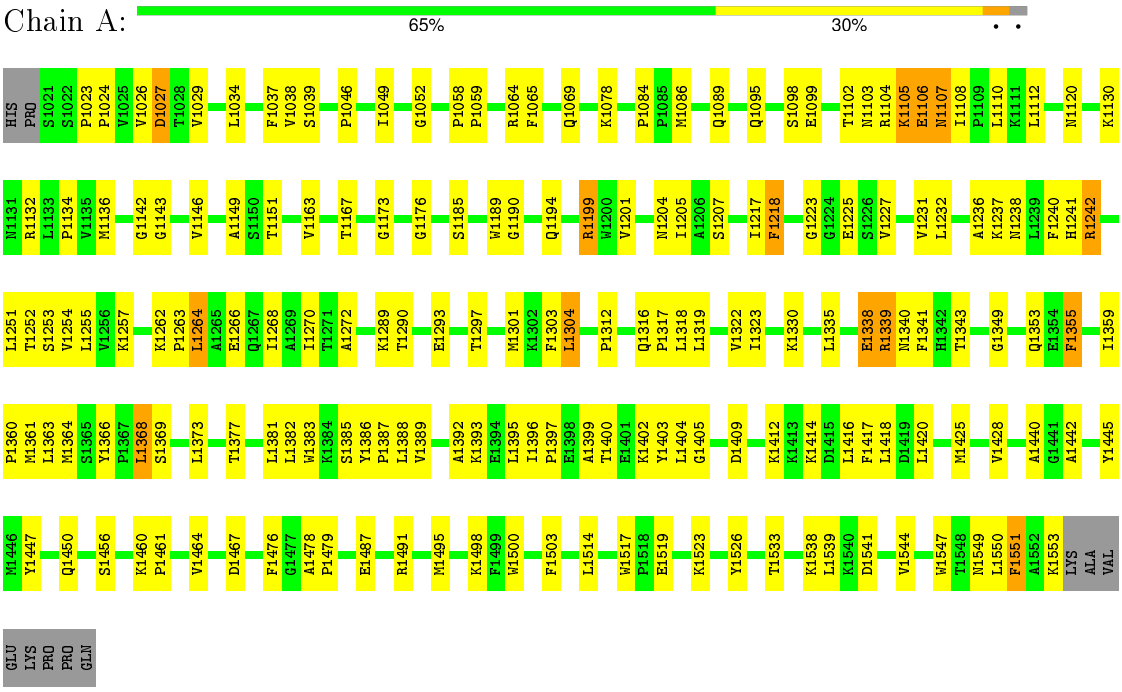
3 Residue-property plots (i)

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.

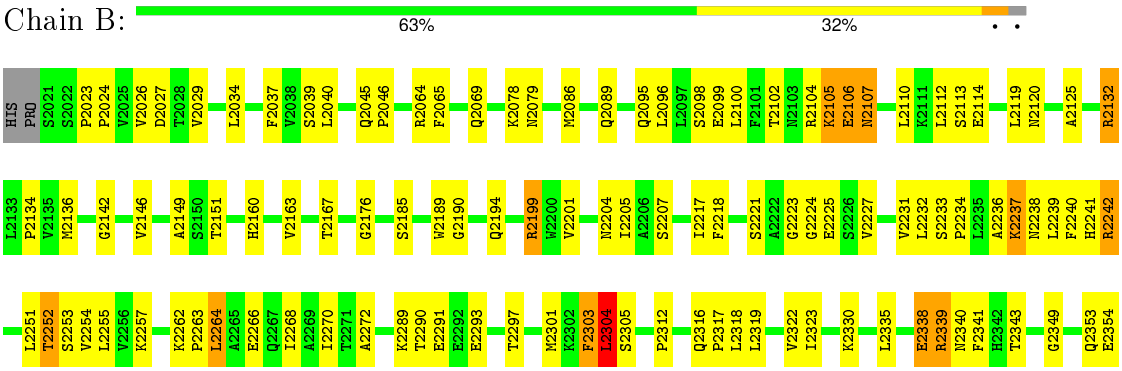
• Molecule 1: Liver carboxylesterase 1

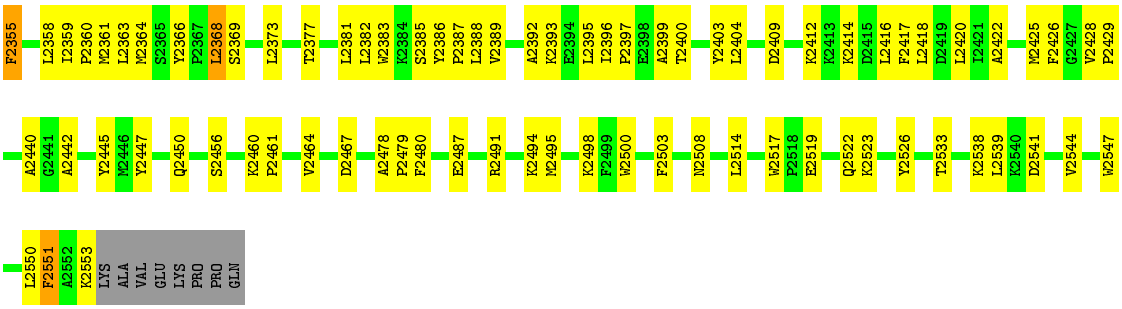
Chain A:



• Molecule 1: Liver carboxylesterase 1

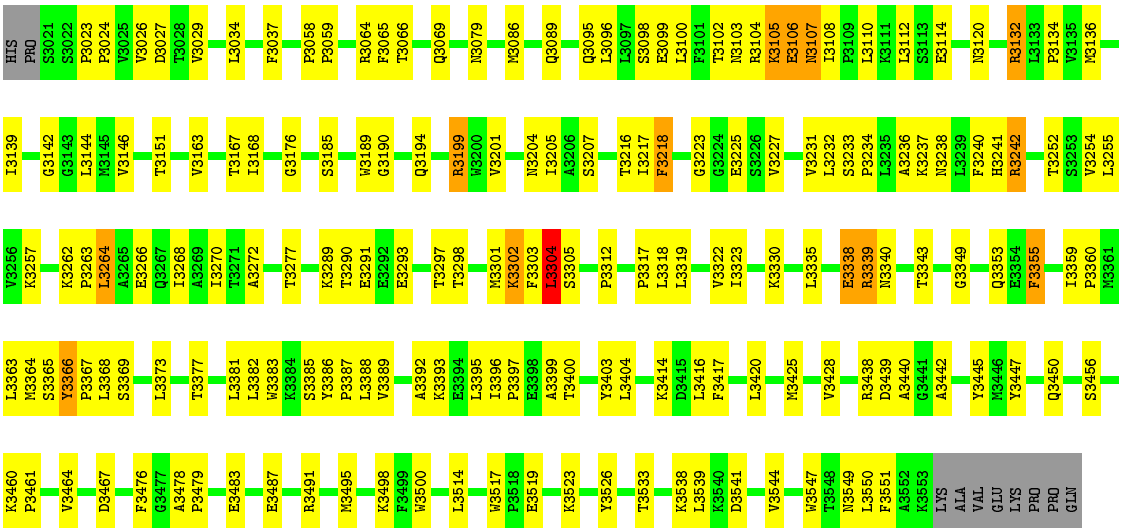
Chain B:





- Molecule 1: Liver carboxylesterase 1

Chain C:



4 Data and refinement statistics (i)

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	55.42Å 179.95Å 201.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.61 – 3.20	Depositor
% Data completeness (in resolution range)	98.6 (30.61-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: TCH, 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	0.49	2/4236 (0.0%)	0.61	0/5754
1	B	0.44	0/4236	0.61	2/5754 (0.0%)
1	C	0.46	1/4236 (0.0%)	0.61	1/5754 (0.0%)
All	All	0.46	3/12708 (0.0%)	0.61	3/17262 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1549	ASN	CG-OD1	-9.65	1.02	1.24
1	A	1549	ASN	CG-ND2	-9.52	1.09	1.32
1	C	3549	ASN	CG-OD1	-5.01	1.12	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2303	PHE	N-CA-C	6.79	129.34	111.00
1	C	3304	LEU	CA-CB-CG	-6.53	100.29	115.30
1	B	2304	LEU	CA-CB-CG	-5.45	102.77	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4130	0	4130	179	0
1	B	4130	0	4131	197	0
1	C	4130	0	4130	210	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	21	0	18	2	0
3	B	21	0	18	6	0
3	C	21	0	18	5	0
4	C	14	0	13	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	1	0
6	A	70	0	87	31	0
6	B	70	0	87	39	0
6	C	70	0	87	48	0
7	A	104	0	0	11	0
7	B	72	0	0	13	0
7	C	77	0	0	11	0
All	All	12988	0	12745	589	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 23.

The worst 5 of 589 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:3252:THR:HG21	6:C:302:TCH:O3	1.33	1.22
1:A:1304:LEU:HD13	6:A:102:TCH:C18	1.69	1.22
1:C:3255:LEU:HG	6:C:302:TCH:H2	1.15	1.13
1:C:3301:MET:HB2	1:C:3303:PHE:CZ	1.87	1.08
1:C:3255:LEU:HG	6:C:302:TCH:C2	1.84	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	530/542 (98%)	473 (89%)	54 (10%)	3 (1%)	30 75
1	B	530/542 (98%)	473 (89%)	53 (10%)	4 (1%)	24 69
1	C	530/542 (98%)	467 (88%)	60 (11%)	3 (1%)	30 75
All	All	1590/1626 (98%)	1413 (89%)	167 (10%)	10 (1%)	30 75

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3302	LYS
1	B	2185	SER
1	C	3185	SER
1	C	3304	LEU
1	A	1185	SER

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	448/457 (98%)	423 (94%)	25 (6%)	26 68
1	B	448/457 (98%)	426 (95%)	22 (5%)	31 72
1	C	448/457 (98%)	425 (95%)	23 (5%)	29 70
All	All	1344/1371 (98%)	1274 (95%)	70 (5%)	29 69

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2132	ARG
1	B	2339	ARG
1	C	3366	TYR
1	B	2151	THR
1	B	2242	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	C	3030	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

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	$\#\|Z\| > 2$
6	TCH	A	101	-	37,38,38	2.62	17 (45%)	59,60,60	3.92	34 (57%)
6	TCH	A	102	-	37,38,38	2.94	17 (45%)	59,60,60	11.49	40 (67%)
2	NAG	A	179	1	14,14,15	0.60	0	15,19,21	0.77	1 (6%)
3	SIA	A	182	-	17,21,21	0.86	0	19,31,31	1.00	2 (10%)
5	SO4	A	184	-	4,4,4	0.22	0	6,6,6	0.14	0
5	SO4	A	284	-	4,4,4	0.44	0	6,6,6	0.21	0
6	TCH	B	201	-	37,38,38	2.69	19 (51%)	59,60,60	3.90	32 (54%)
6	TCH	B	202	-	37,38,38	2.98	15 (40%)	59,60,60	11.42	40 (67%)
2	NAG	B	279	1	14,14,15	0.84	1 (7%)	15,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SIA	B	282	-	17,21,21	0.90	1 (5%)	19,31,31	1.02	0
5	SO4	B	285	-	4,4,4	0.40	0	6,6,6	0.16	0
5	SO4	B	385	-	4,4,4	0.39	0	6,6,6	0.28	0
5	SO4	C	185	-	4,4,4	0.43	0	6,6,6	0.17	0
6	TCH	C	301	-	37,38,38	2.70	17 (45%)	59,60,60	3.92	36 (61%)
6	TCH	C	302	-	37,38,38	3.31	18 (48%)	59,60,60	11.40	41 (69%)
4	NDG	C	379	1	14,14,15	0.75	0	15,19,21	0.88	1 (6%)
3	SIA	C	382	-	17,21,21	0.99	1 (5%)	19,31,31	0.91	2 (10%)
5	SO4	C	384	-	4,4,4	0.37	0	6,6,6	0.21	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	TCH	A	101	-	4/4/13/14	2/16/81/81	0/4/4/4
6	TCH	A	102	-	4/4/13/14	0/16/81/81	0/4/4/4
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
5	SO4	A	184	-	-	0/0/0/0	0/0/0/0
5	SO4	A	284	-	-	0/0/0/0	0/0/0/0
6	TCH	B	201	-	4/4/13/14	2/16/81/81	0/4/4/4
6	TCH	B	202	-	4/4/13/14	0/16/81/81	0/4/4/4
2	NAG	B	279	1	-	0/6/23/26	0/1/1/1
3	SIA	B	282	-	-	0/14/38/38	0/1/1/1
5	SO4	B	285	-	-	0/0/0/0	0/0/0/0
5	SO4	B	385	-	-	0/0/0/0	0/0/0/0
5	SO4	C	185	-	-	0/0/0/0	0/0/0/0
6	TCH	C	301	-	4/4/13/14	1/16/81/81	0/4/4/4
6	TCH	C	302	-	4/4/13/14	0/16/81/81	0/4/4/4
4	NDG	C	379	1	-	0/6/23/26	0/1/1/1
3	SIA	C	382	-	-	1/14/38/38	0/1/1/1
5	SO4	C	384	-	-	0/0/0/0	0/0/0/0

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	TCH	O3S-S26	-7.04	1.28	1.46
6	C	302	TCH	O3S-S26	-6.74	1.29	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	102	TCH	O3S-S26	-6.70	1.29	1.46
6	B	202	TCH	C25-N24	-5.00	1.34	1.46
6	C	302	TCH	C6-C5	-4.74	1.45	1.53

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	302	TCH	O1S-S26-C26	-21.96	88.17	106.91
6	A	102	TCH	O1S-S26-C26	-21.26	88.76	106.91
6	B	202	TCH	O1S-S26-C26	-20.22	89.66	106.91
6	A	102	TCH	O3S-S26-O2S	-13.68	79.78	111.61
6	C	302	TCH	O3S-S26-O2S	-13.56	80.06	111.61

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	302	TCH	C5
6	C	302	TCH	C3
6	C	302	TCH	C20
6	C	302	TCH	C9
6	B	201	TCH	C5

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	382	SIA	O10-C10-N5-C5
6	A	101	TCH	C23-C24-N24-C25
6	B	201	TCH	C23-C24-N24-C25
6	C	301	TCH	S26-C26-C25-N24
6	A	101	TCH	S26-C26-C25-N24

There are no ring outliers.

11 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	101	TCH	5	0
6	A	102	TCH	26	0
2	A	179	NAG	1	0
3	A	182	SIA	2	0
6	B	201	TCH	5	0
6	B	202	TCH	34	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	282	SIA	6	0
5	C	185	SO4	1	0
6	C	301	TCH	7	0
6	C	302	TCH	41	0
3	C	382	SIA	5	0

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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