



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2016 – 06:47 PM EST

PDB ID : 1WND
Title : Escherichia coli YdcW gene product is a medium-chain aldehyde dehydrogenase as determined by kinetics and crystal structure
Authors : Gruez, A.; Roig-Zamboni, V.; Tegoni, M.; Cambillau, C.
Deposited on : 2004-07-29
Resolution : 2.10 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

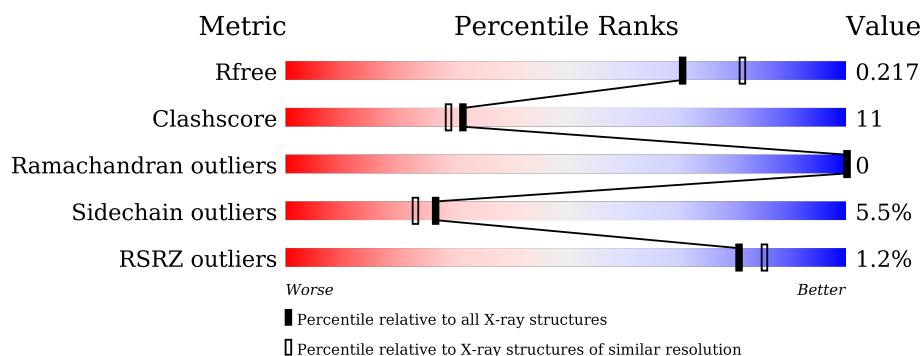
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	495	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>.</div> <div>.</div> </div> </div>
1	B	495	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>.</div> <div>.</div> </div> </div>
1	C	495	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>.</div> <div>.</div> </div> </div>
1	D	495	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14574 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 Putative betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	85	0	0
			3575	2263	616	679	17			
1	B	474	Total	C	N	O	S	54	0	0
			3575	2263	616	679	17			
1	C	474	Total	C	N	O	S	59	0	0
			3575	2263	616	679	17			
1	D	474	Total	C	N	O	S	52	0	0
			3575	2263	616	679	17			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	EXPRESSION TAG	UNP P77674
A	-19	TYR	-	EXPRESSION TAG	UNP P77674
A	-18	TYR	-	EXPRESSION TAG	UNP P77674
A	-17	HIS	-	EXPRESSION TAG	UNP P77674
A	-16	HIS	-	EXPRESSION TAG	UNP P77674
A	-15	HIS	-	EXPRESSION TAG	UNP P77674
A	-14	HIS	-	EXPRESSION TAG	UNP P77674
A	-13	HIS	-	EXPRESSION TAG	UNP P77674
A	-12	HIS	-	EXPRESSION TAG	UNP P77674
A	-11	LEU	-	EXPRESSION TAG	UNP P77674
A	-10	GLU	-	EXPRESSION TAG	UNP P77674
A	-9	SER	-	EXPRESSION TAG	UNP P77674
A	-8	THR	-	EXPRESSION TAG	UNP P77674
A	-7	SER	-	EXPRESSION TAG	UNP P77674
A	-6	LEU	-	EXPRESSION TAG	UNP P77674
A	-5	TYR	-	EXPRESSION TAG	UNP P77674
A	-4	LYS	-	EXPRESSION TAG	UNP P77674
A	-3	LYS	-	EXPRESSION TAG	UNP P77674
A	-2	ALA	-	EXPRESSION TAG	UNP P77674
A	-1	GLY	-	EXPRESSION TAG	UNP P77674
A	0	LEU	-	EXPRESSION TAG	UNP P77674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	VAL	ILE	CONFLICT	UNP P77674
B	-20	SER	-	EXPRESSION TAG	UNP P77674
B	-19	TYR	-	EXPRESSION TAG	UNP P77674
B	-18	TYR	-	EXPRESSION TAG	UNP P77674
B	-17	HIS	-	EXPRESSION TAG	UNP P77674
B	-16	HIS	-	EXPRESSION TAG	UNP P77674
B	-15	HIS	-	EXPRESSION TAG	UNP P77674
B	-14	HIS	-	EXPRESSION TAG	UNP P77674
B	-13	HIS	-	EXPRESSION TAG	UNP P77674
B	-12	HIS	-	EXPRESSION TAG	UNP P77674
B	-11	LEU	-	EXPRESSION TAG	UNP P77674
B	-10	GLU	-	EXPRESSION TAG	UNP P77674
B	-9	SER	-	EXPRESSION TAG	UNP P77674
B	-8	THR	-	EXPRESSION TAG	UNP P77674
B	-7	SER	-	EXPRESSION TAG	UNP P77674
B	-6	LEU	-	EXPRESSION TAG	UNP P77674
B	-5	TYR	-	EXPRESSION TAG	UNP P77674
B	-4	LYS	-	EXPRESSION TAG	UNP P77674
B	-3	LYS	-	EXPRESSION TAG	UNP P77674
B	-2	ALA	-	EXPRESSION TAG	UNP P77674
B	-1	GLY	-	EXPRESSION TAG	UNP P77674
B	0	LEU	-	EXPRESSION TAG	UNP P77674
B	197	VAL	ILE	CONFLICT	UNP P77674
C	-20	SER	-	EXPRESSION TAG	UNP P77674
C	-19	TYR	-	EXPRESSION TAG	UNP P77674
C	-18	TYR	-	EXPRESSION TAG	UNP P77674
C	-17	HIS	-	EXPRESSION TAG	UNP P77674
C	-16	HIS	-	EXPRESSION TAG	UNP P77674
C	-15	HIS	-	EXPRESSION TAG	UNP P77674
C	-14	HIS	-	EXPRESSION TAG	UNP P77674
C	-13	HIS	-	EXPRESSION TAG	UNP P77674
C	-12	HIS	-	EXPRESSION TAG	UNP P77674
C	-11	LEU	-	EXPRESSION TAG	UNP P77674
C	-10	GLU	-	EXPRESSION TAG	UNP P77674
C	-9	SER	-	EXPRESSION TAG	UNP P77674
C	-8	THR	-	EXPRESSION TAG	UNP P77674
C	-7	SER	-	EXPRESSION TAG	UNP P77674
C	-6	LEU	-	EXPRESSION TAG	UNP P77674
C	-5	TYR	-	EXPRESSION TAG	UNP P77674
C	-4	LYS	-	EXPRESSION TAG	UNP P77674
C	-3	LYS	-	EXPRESSION TAG	UNP P77674
C	-2	ALA	-	EXPRESSION TAG	UNP P77674

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P77674
C	0	LEU	-	EXPRESSION TAG	UNP P77674
C	197	VAL	ILE	CONFLICT	UNP P77674
D	-20	SER	-	EXPRESSION TAG	UNP P77674
D	-19	TYR	-	EXPRESSION TAG	UNP P77674
D	-18	TYR	-	EXPRESSION TAG	UNP P77674
D	-17	HIS	-	EXPRESSION TAG	UNP P77674
D	-16	HIS	-	EXPRESSION TAG	UNP P77674
D	-15	HIS	-	EXPRESSION TAG	UNP P77674
D	-14	HIS	-	EXPRESSION TAG	UNP P77674
D	-13	HIS	-	EXPRESSION TAG	UNP P77674
D	-12	HIS	-	EXPRESSION TAG	UNP P77674
D	-11	LEU	-	EXPRESSION TAG	UNP P77674
D	-10	GLU	-	EXPRESSION TAG	UNP P77674
D	-9	SER	-	EXPRESSION TAG	UNP P77674
D	-8	THR	-	EXPRESSION TAG	UNP P77674
D	-7	SER	-	EXPRESSION TAG	UNP P77674
D	-6	LEU	-	EXPRESSION TAG	UNP P77674
D	-5	TYR	-	EXPRESSION TAG	UNP P77674
D	-4	LYS	-	EXPRESSION TAG	UNP P77674
D	-3	LYS	-	EXPRESSION TAG	UNP P77674
D	-2	ALA	-	EXPRESSION TAG	UNP P77674
D	-1	GLY	-	EXPRESSION TAG	UNP P77674
D	0	LEU	-	EXPRESSION TAG	UNP P77674
D	197	VAL	ILE	CONFLICT	UNP P77674

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

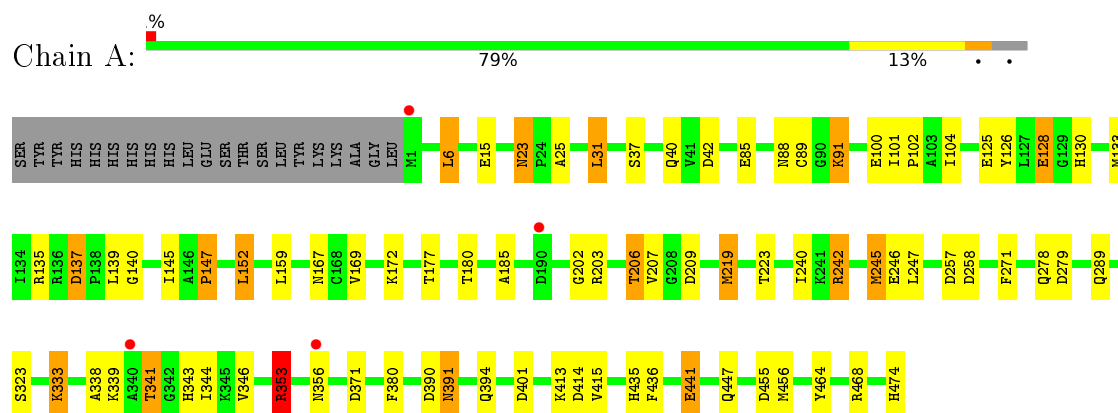
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total 67	O 67	0	0
3	B	65	Total 65	O 65	0	0
3	C	66	Total 66	O 66	0	0
3	D	72	Total 72	O 72	0	0

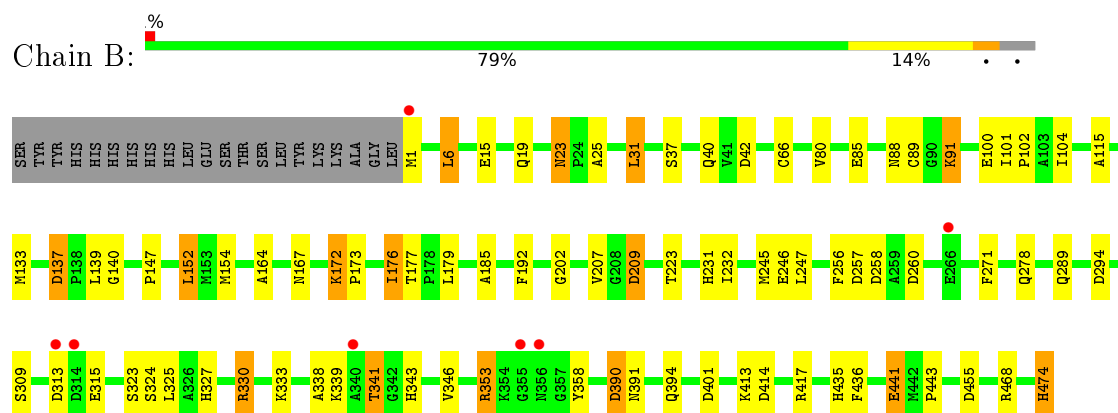
3 Residue-property plots

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.

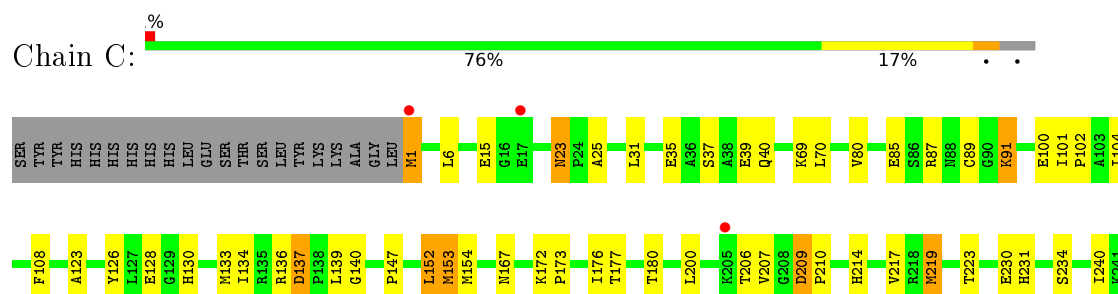
- Molecule 1: Putative betaine aldehyde dehydrogenase

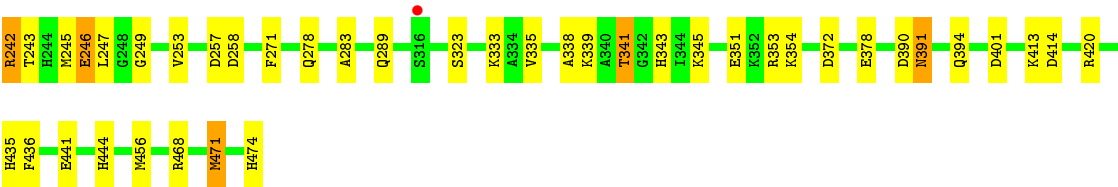


- Molecule 1: Putative betaine aldehyde dehydrogenase

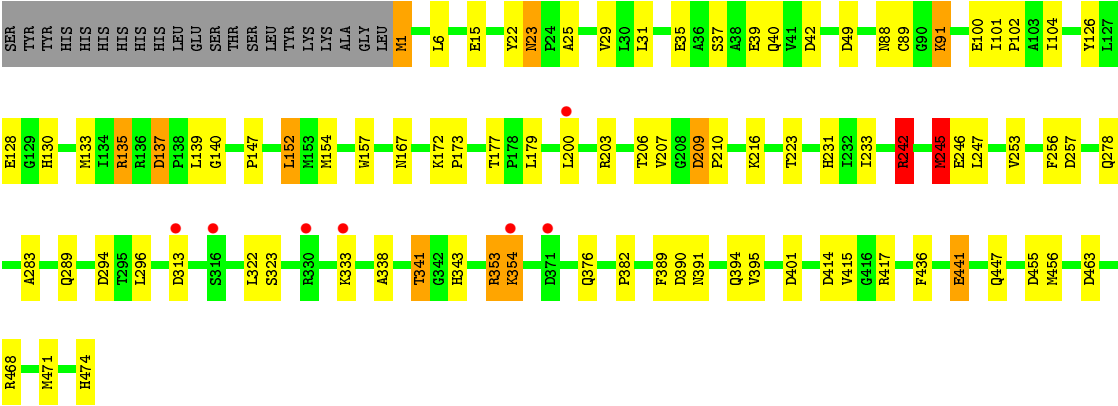
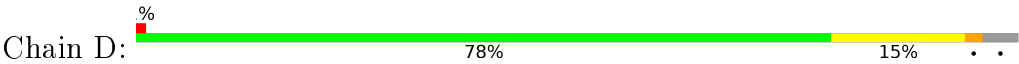


- Molecule 1: Putative betaine aldehyde dehydrogenase





● Molecule 1: Putative betaine aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.04Å 79.68Å 158.67Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 98.8 (19.94-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.184 , 0.213 0.191 , 0.217	Depositor DCC
R_{free} test set	6119 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14574	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA

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	0.65	0/3649	0.86	12/4955 (0.2%)
1	B	0.62	0/3649	0.83	13/4955 (0.3%)
1	C	0.63	0/3649	0.85	11/4955 (0.2%)
1	D	0.65	1/3649 (0.0%)	0.85	14/4955 (0.3%)
All	All	0.64	1/14596 (0.0%)	0.85	50/19820 (0.3%)

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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	245	MET	C-N	6.01	1.47	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	MET	CA-C-N	-8.68	98.11	117.20
1	A	353	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	242	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	A	137	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	353	ARG	NE-CZ-NH2	7.32	123.96	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain
1	B	353	ARG	Sidechain
1	D	245	MET	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	3575	0	3558	78	0
1	B	3575	0	3558	75	0
1	C	3575	0	3558	90	0
1	D	3575	0	3558	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	67	0	0	0	0
3	B	65	0	0	5	0
3	C	66	0	0	4	0
3	D	72	0	0	2	0
All	All	14574	0	14232	300	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 11.

The worst 5 of 300 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:242:ARG:NH1	1:C:243:THR:H	1.39	1.20
1:B:474:HIS:OXT	1:B:474:HIS:CD2	1.96	1.18
1:A:139:LEU:CD1	1:A:219:MET:CE	2.23	1.17
1:B:330:ARG:HH11	1:B:330:ARG:HG2	1.05	1.14
1:A:245:MET:HG2	1:A:247:LEU:HD21	1.19	1.12

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	472/495 (95%)	464 (98%)	8 (2%)	0	100	100
1	B	472/495 (95%)	462 (98%)	10 (2%)	0	100	100
1	C	472/495 (95%)	463 (98%)	9 (2%)	0	100	100
1	D	472/495 (95%)	461 (98%)	11 (2%)	0	100	100
All	All	1888/1980 (95%)	1850 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	371/390 (95%)	348 (94%)	23 (6%)	23	19
1	B	371/390 (95%)	354 (95%)	17 (5%)	33	31
1	C	371/390 (95%)	348 (94%)	23 (6%)	23	19
1	D	371/390 (95%)	353 (95%)	18 (5%)	31	28
All	All	1484/1560 (95%)	1403 (94%)	81 (6%)	27	23

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

Mol	Chain	Res	Type
1	B	333	LYS
1	C	69	LYS
1	D	246	GLU
1	B	341	THR
1	C	6	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	419	HIS
1	C	167	ASN
1	D	376	GLN
1	C	23	ASN
1	C	278	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/495 (95%)	-0.20	4 (0%) 87 90	13, 20, 27, 35	21 (4%)
1	B	474/495 (95%)	-0.20	7 (1%) 76 81	14, 20, 27, 35	13 (2%)
1	C	474/495 (95%)	-0.19	4 (0%) 87 90	14, 20, 27, 36	15 (3%)
1	D	474/495 (95%)	-0.19	7 (1%) 76 81	14, 20, 27, 39	13 (2%)
All	All	1896/1980 (95%)	-0.19	22 (1%) 81 85	13, 20, 27, 39	62 (3%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.6
1	D	313	ASP	3.2
1	D	354	LYS	3.2
1	B	314	ASP	2.8
1	B	266	GLU	2.8

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	475	1/1	0.99	0.05	-2.50	27,27,27,27	0
2	CA	C	475	1/1	1.00	0.04	-2.70	26,26,26,26	0
2	CA	D	475	1/1	0.99	0.05	-3.37	26,26,26,26	0
2	CA	A	475	1/1	0.99	0.03	-4.29	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.