Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 03:19 AM EDT

PDB ID	:	4QTO
Title	:	1.65 Angstrom resolution crystal structure of betaine aldehyde dehydrogenase (betB) from Staphylococcus aureus with BME-modified Cys289 and PEG molecule in active site
Authors	:	Halavaty, A.S.; Minasov, G.; Dubrovska, I.; Winsor, J.; Shuvalova, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2014-07-08
Resolution	:	1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

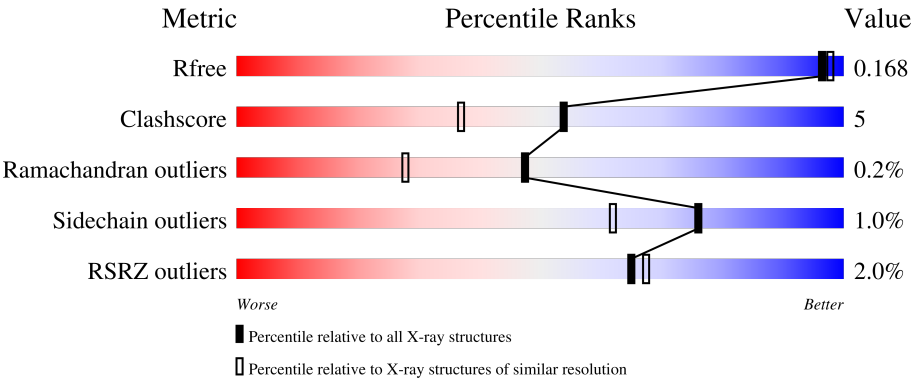
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	520	2% 87% 8% •
1	B	520	3% 87% 7% • •
1	C	520	% 87% 7% • 5%
1	D	520	% 88% 7% • 5%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19380 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 Betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	34	0
			4145	2611	699	815	20			
1	B	497	Total	C	N	O	S	0	33	0
			4124	2596	695	814	19			
1	C	496	Total	C	N	O	S	0	38	0
			4161	2620	707	814	20			
1	D	495	Total	C	N	O	S	0	28	0
			4079	2568	690	803	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q5HCU0
A	-22	HIS	-	expression tag	UNP Q5HCU0
A	-21	HIS	-	expression tag	UNP Q5HCU0
A	-20	HIS	-	expression tag	UNP Q5HCU0
A	-19	HIS	-	expression tag	UNP Q5HCU0
A	-18	HIS	-	expression tag	UNP Q5HCU0
A	-17	HIS	-	expression tag	UNP Q5HCU0
A	-16	SER	-	expression tag	UNP Q5HCU0
A	-15	SER	-	expression tag	UNP Q5HCU0
A	-14	GLY	-	expression tag	UNP Q5HCU0
A	-13	VAL	-	expression tag	UNP Q5HCU0
A	-12	ASP	-	expression tag	UNP Q5HCU0
A	-11	LEU	-	expression tag	UNP Q5HCU0
A	-10	GLY	-	expression tag	UNP Q5HCU0
A	-9	THR	-	expression tag	UNP Q5HCU0
A	-8	GLU	-	expression tag	UNP Q5HCU0
A	-7	ASN	-	expression tag	UNP Q5HCU0
A	-6	LEU	-	expression tag	UNP Q5HCU0
A	-5	TYR	-	expression tag	UNP Q5HCU0
A	-4	PHE	-	expression tag	UNP Q5HCU0
A	-3	GLN	-	expression tag	UNP Q5HCU0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5HCU0
A	-1	ASN	-	expression tag	UNP Q5HCU0
A	0	ALA	-	expression tag	UNP Q5HCU0
B	-23	MET	-	expression tag	UNP Q5HCU0
B	-22	HIS	-	expression tag	UNP Q5HCU0
B	-21	HIS	-	expression tag	UNP Q5HCU0
B	-20	HIS	-	expression tag	UNP Q5HCU0
B	-19	HIS	-	expression tag	UNP Q5HCU0
B	-18	HIS	-	expression tag	UNP Q5HCU0
B	-17	HIS	-	expression tag	UNP Q5HCU0
B	-16	SER	-	expression tag	UNP Q5HCU0
B	-15	SER	-	expression tag	UNP Q5HCU0
B	-14	GLY	-	expression tag	UNP Q5HCU0
B	-13	VAL	-	expression tag	UNP Q5HCU0
B	-12	ASP	-	expression tag	UNP Q5HCU0
B	-11	LEU	-	expression tag	UNP Q5HCU0
B	-10	GLY	-	expression tag	UNP Q5HCU0
B	-9	THR	-	expression tag	UNP Q5HCU0
B	-8	GLU	-	expression tag	UNP Q5HCU0
B	-7	ASN	-	expression tag	UNP Q5HCU0
B	-6	LEU	-	expression tag	UNP Q5HCU0
B	-5	TYR	-	expression tag	UNP Q5HCU0
B	-4	PHE	-	expression tag	UNP Q5HCU0
B	-3	GLN	-	expression tag	UNP Q5HCU0
B	-2	SER	-	expression tag	UNP Q5HCU0
B	-1	ASN	-	expression tag	UNP Q5HCU0
B	0	ALA	-	expression tag	UNP Q5HCU0
C	-23	MET	-	expression tag	UNP Q5HCU0
C	-22	HIS	-	expression tag	UNP Q5HCU0
C	-21	HIS	-	expression tag	UNP Q5HCU0
C	-20	HIS	-	expression tag	UNP Q5HCU0
C	-19	HIS	-	expression tag	UNP Q5HCU0
C	-18	HIS	-	expression tag	UNP Q5HCU0
C	-17	HIS	-	expression tag	UNP Q5HCU0
C	-16	SER	-	expression tag	UNP Q5HCU0
C	-15	SER	-	expression tag	UNP Q5HCU0
C	-14	GLY	-	expression tag	UNP Q5HCU0
C	-13	VAL	-	expression tag	UNP Q5HCU0
C	-12	ASP	-	expression tag	UNP Q5HCU0
C	-11	LEU	-	expression tag	UNP Q5HCU0
C	-10	GLY	-	expression tag	UNP Q5HCU0
C	-9	THR	-	expression tag	UNP Q5HCU0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q5HCU0
C	-7	ASN	-	expression tag	UNP Q5HCU0
C	-6	LEU	-	expression tag	UNP Q5HCU0
C	-5	TYR	-	expression tag	UNP Q5HCU0
C	-4	PHE	-	expression tag	UNP Q5HCU0
C	-3	GLN	-	expression tag	UNP Q5HCU0
C	-2	SER	-	expression tag	UNP Q5HCU0
C	-1	ASN	-	expression tag	UNP Q5HCU0
C	0	ALA	-	expression tag	UNP Q5HCU0
D	-23	MET	-	expression tag	UNP Q5HCU0
D	-22	HIS	-	expression tag	UNP Q5HCU0
D	-21	HIS	-	expression tag	UNP Q5HCU0
D	-20	HIS	-	expression tag	UNP Q5HCU0
D	-19	HIS	-	expression tag	UNP Q5HCU0
D	-18	HIS	-	expression tag	UNP Q5HCU0
D	-17	HIS	-	expression tag	UNP Q5HCU0
D	-16	SER	-	expression tag	UNP Q5HCU0
D	-15	SER	-	expression tag	UNP Q5HCU0
D	-14	GLY	-	expression tag	UNP Q5HCU0
D	-13	VAL	-	expression tag	UNP Q5HCU0
D	-12	ASP	-	expression tag	UNP Q5HCU0
D	-11	LEU	-	expression tag	UNP Q5HCU0
D	-10	GLY	-	expression tag	UNP Q5HCU0
D	-9	THR	-	expression tag	UNP Q5HCU0
D	-8	GLU	-	expression tag	UNP Q5HCU0
D	-7	ASN	-	expression tag	UNP Q5HCU0
D	-6	LEU	-	expression tag	UNP Q5HCU0
D	-5	TYR	-	expression tag	UNP Q5HCU0
D	-4	PHE	-	expression tag	UNP Q5HCU0
D	-3	GLN	-	expression tag	UNP Q5HCU0
D	-2	SER	-	expression tag	UNP Q5HCU0
D	-1	ASN	-	expression tag	UNP Q5HCU0
D	0	ALA	-	expression tag	UNP Q5HCU0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

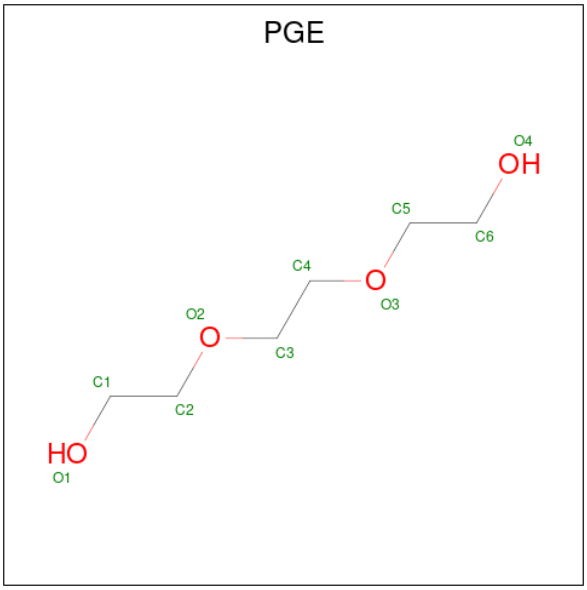
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

Continued on next page...

Continued from previous page...

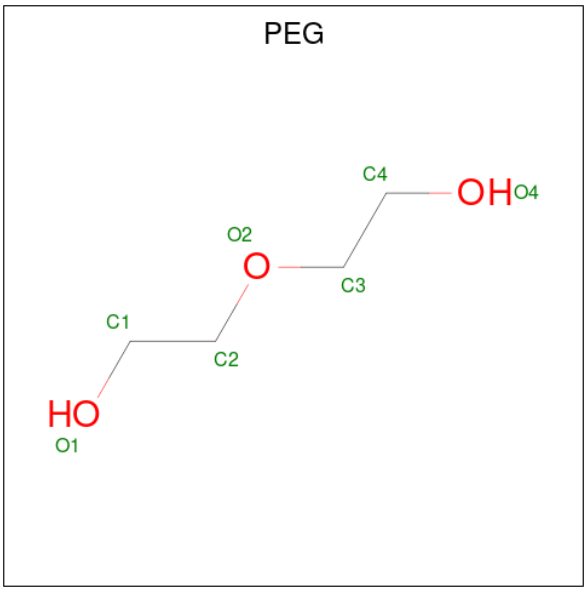
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Na 1 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



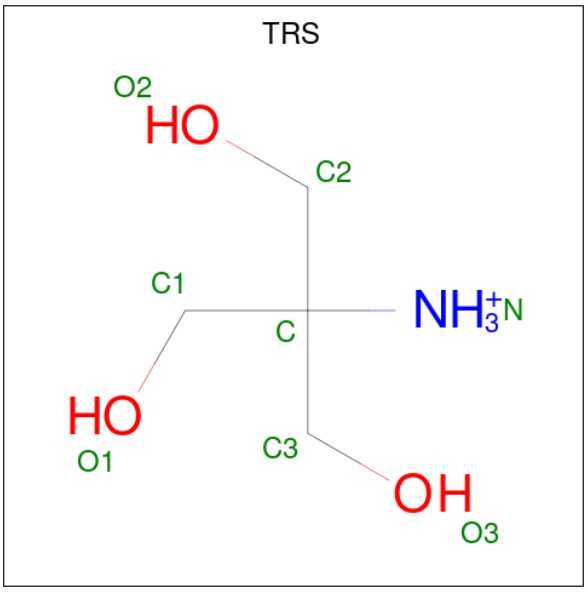
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 10 6 4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



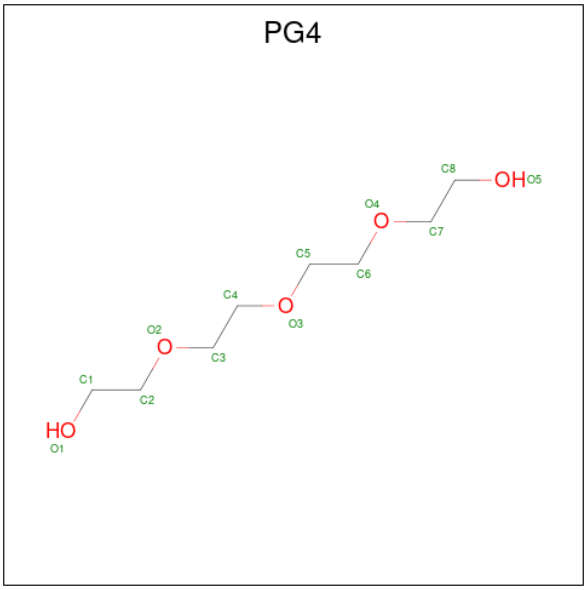
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



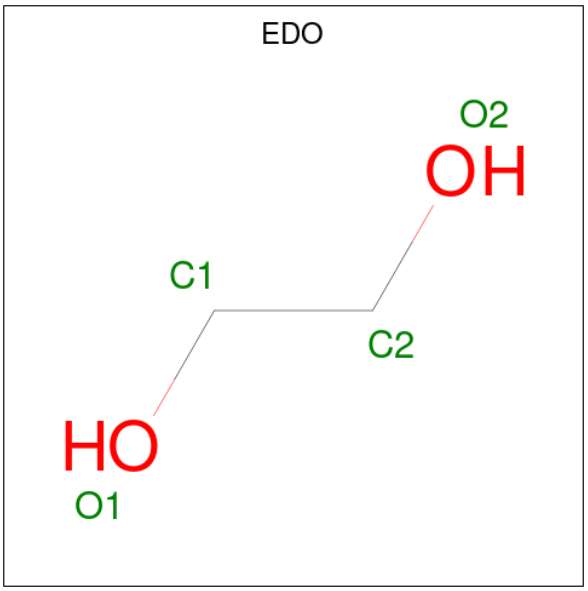
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0
5	B	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 13 8 5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	1

- Molecule 8 is water.

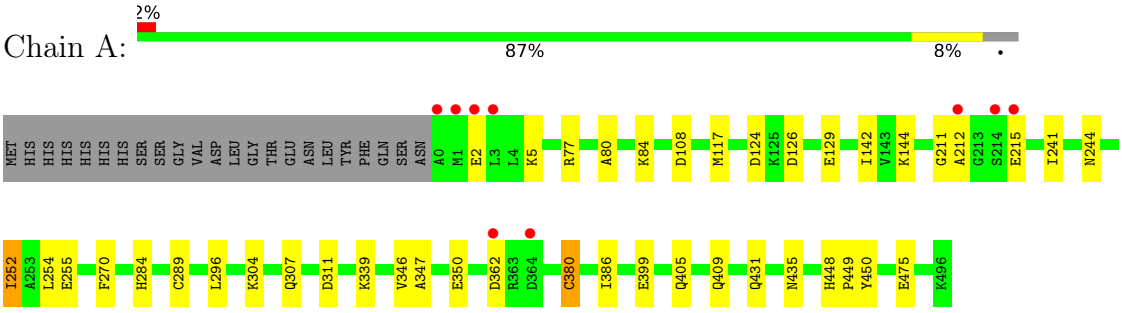
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	677	Total O 700 700	0	36
8	B	646	Total O 662 662	0	29
8	C	664	Total O 685 685	0	31
8	D	676	Total O 695 695	0	25

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

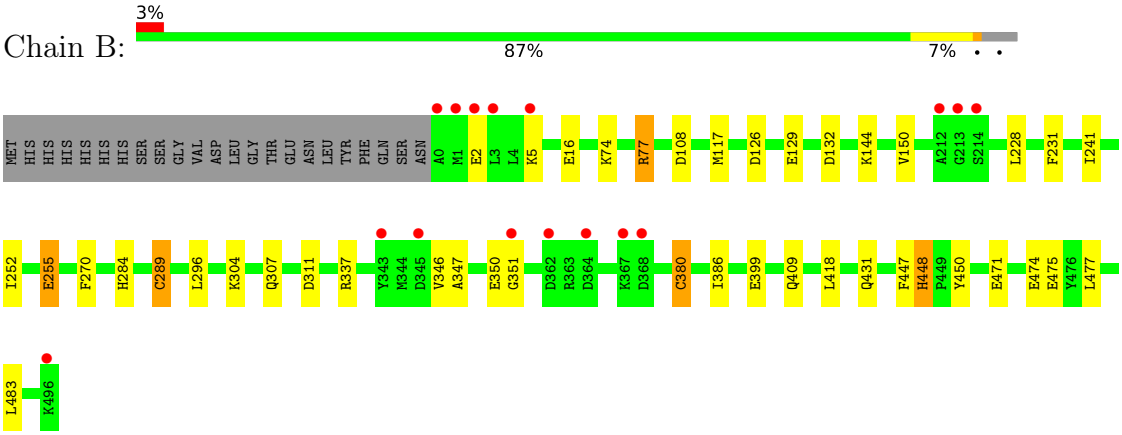
• Molecule 1: Betaine aldehyde dehydrogenase

Chain A:



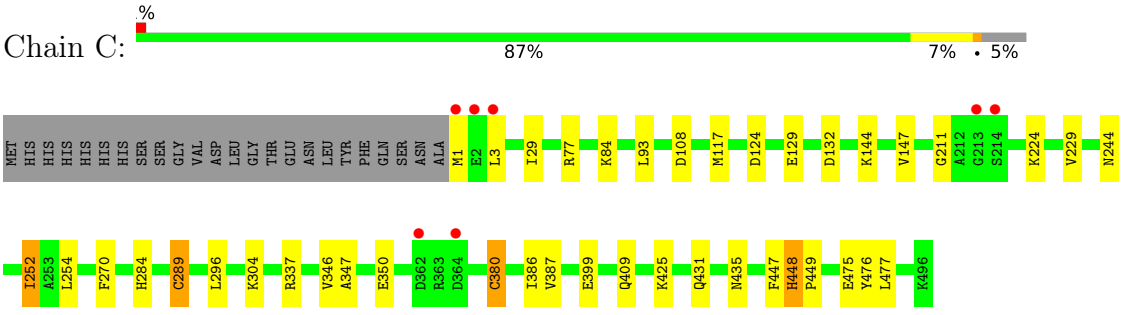
• Molecule 1: Betaine aldehyde dehydrogenase

Chain B:



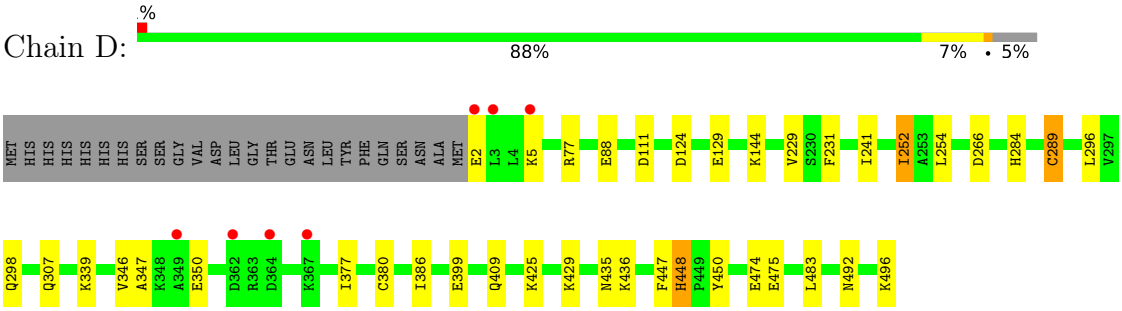
• Molecule 1: Betaine aldehyde dehydrogenase

Chain C:



• Molecule 1: Betaine aldehyde dehydrogenase

Chain D:


%
88%
7%
5%
MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER ASN ALA MET E2 L3 L4 K5 R77 E88 D111 D124 E129 K144 V229 S230 F231 I241 I252 A253 L254 D266 H284 C289 L296 V297
Q298 Q307 K339 V346 A347 K348 A349 E350 D362 R363 D364 K367 I377 C380 I386 E399 Q409 K425 K429 N435 K436 F447 H448 P449 Y450 E474 E475 L483 N492 K496

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.25Å 102.47Å 118.18Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	29.71 – 1.65 29.69 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.71-1.65) 98.6 (29.69-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.136 , 0.156 0.150 , 0.168	Depositor DCC
R_{free} test set	15433 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19380	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TRS, PG4, EDO, PGE, CME, PEG

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	0.60	0/4196	0.81	3/5667 (0.1%)
1	B	0.58	0/4177	0.80	5/5645 (0.1%)
1	C	0.57	0/4212	0.79	5/5688 (0.1%)
1	D	0.57	0/4132	0.78	0/5585
All	All	0.58	0/16717	0.80	13/22585 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	380[A]	CYS	CA-CB-SG	6.40	125.52	114.00
1	A	380[B]	CYS	CA-CB-SG	6.40	125.52	114.00
1	B	108	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	108	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	C	337	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	108	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	C	337	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	380[A]	CYS	CA-CB-SG	5.49	123.88	114.00
1	C	380[B]	CYS	CA-CB-SG	5.49	123.88	114.00
1	B	380[A]	CYS	CA-CB-SG	5.41	123.73	114.00
1	B	380[B]	CYS	CA-CB-SG	5.41	123.73	114.00
1	B	337	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	337	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	4145	0	4075	41	0
1	B	4124	0	4047	53	0
1	C	4161	0	4097	46	0
1	D	4079	0	3991	40	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	20	0	28	0	0
3	B	10	0	14	0	0
3	C	10	0	14	1	0
3	D	10	0	14	1	0
4	A	21	0	30	2	0
4	B	14	0	20	1	0
4	D	7	0	10	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
6	C	13	0	18	0	0
7	C	4	0	6	3	0
8	A	700	0	0	24	0
8	B	662	0	0	23	0
8	C	685	0	0	26	0
8	D	695	0	0	18	0
All	All	19380	0	16388	177	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 5.

All (177) 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:450[B]:TYR:HE2	8:B:951:HOH:O	1.32	1.10
8:C:1237:HOH:O	1:D:474:GLU:HG3	1.51	1.09
1:D:450[A]:TYR:HE2	8:D:1252:HOH:O	1.38	1.07
1:A:450[B]:TYR:HE1	8:A:729:HOH:O	1.39	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77[B]:ARG:NH1	1:C:117[B]:MET:CE	2.25	1.00
1:C:29[B]:ILE:HD11	8:C:890:HOH:O	1.65	0.96
1:B:77[B]:ARG:NH1	1:C:117[B]:MET:HE1	1.85	0.91
1:A:212:ALA:HB3	1:A:215[B]:GLU:HG2	1.52	0.91
1:A:211:GLY:HA3	8:A:1099[B]:HOH:O	1.76	0.84
1:C:475:GLU:HG3	8:C:914:HOH:O	1.75	0.84
1:D:229[B]:VAL:HG13	1:D:252[B]:ILE:HD12	1.59	0.83
1:A:126[A]:ASP:HB3	8:A:1277[A]:HOH:O	1.79	0.82
1:C:211:GLY:HA3	8:C:880:HOH:O	1.80	0.81
1:A:311:ASP:HB3	8:A:1213:HOH:O	1.80	0.80
1:B:126[A]:ASP:HB3	8:B:1246[A]:HOH:O	1.82	0.79
1:C:129:GLU:HG3	8:C:1220:HOH:O	1.82	0.78
1:D:2:GLU:O	1:D:5:LYS:HG2	1.85	0.76
1:A:212:ALA:HB3	1:A:215[B]:GLU:CG	2.15	0.76
1:B:2:GLU:O	1:B:5:LYS:HG2	1.84	0.76
1:B:307[A]:GLN:HG2	8:B:959:HOH:O	1.85	0.76
1:A:475:GLU:HG3	8:A:844:HOH:O	1.86	0.75
1:A:2:GLU:O	1:A:5:LYS:HG2	1.86	0.75
1:B:77[B]:ARG:NH1	1:C:117[B]:MET:HE2	2.01	0.74
1:D:347:ALA:HB2	1:D:386[B]:ILE:HG21	1.71	0.72
1:D:77[B]:ARG:NH2	8:D:849:HOH:O	2.22	0.72
1:A:431[B]:GLN:NE2	8:A:1210:HOH:O	2.24	0.71
1:D:129:GLU:HG3	8:D:1269:HOH:O	1.90	0.71
1:B:307[B]:GLN:NE2	1:B:311[B]:ASP:OD1	2.24	0.70
1:A:77[A]:ARG:NH2	8:A:902:HOH:O	2.22	0.70
1:A:347:ALA:HA	1:A:386[B]:ILE:HG21	1.74	0.69
1:D:307:GLN:HG2	8:D:893:HOH:O	1.91	0.69
1:B:475:GLU:HG3	8:B:896:HOH:O	1.93	0.69
1:A:347:ALA:CA	1:A:386[B]:ILE:HG21	2.24	0.68
1:A:84:LYS:NZ	8:A:891:HOH:O	2.26	0.68
1:B:311[B]:ASP:HB3	8:B:920[B]:HOH:O	1.93	0.68
1:C:244[A]:ASN:ND2	8:C:941:HOH:O	2.25	0.68
1:B:409[A]:GLN:HG2	8:B:888:HOH:O	1.93	0.68
1:B:351:GLY:C	8:B:954:HOH:O	2.32	0.67
1:D:475:GLU:HG3	8:D:1133:HOH:O	1.94	0.67
1:C:229[B]:VAL:HG13	1:C:252[B]:ILE:HD12	1.78	0.66
1:C:347:ALA:HB2	1:C:386[B]:ILE:HG21	1.78	0.66
1:C:147[B]:VAL:HG13	1:C:476:TYR:C	2.16	0.66
1:B:77[B]:ARG:CZ	1:C:117[B]:MET:CE	2.74	0.66
1:C:93[B]:LEU:HD12	8:C:888:HOH:O	1.95	0.65
1:C:3:LEU:HB3	8:C:958:HOH:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77[B]:ARG:CZ	1:C:117[B]:MET:HE1	2.28	0.64
1:D:347:ALA:CB	1:D:386[B]:ILE:HG21	2.27	0.63
1:C:289[A]:CME:HZ3	8:C:1261[A]:HOH:O	1.97	0.63
4:A:504:PEG:H22	8:A:1235:HOH:O	1.97	0.63
8:A:992:HOH:O	1:C:124:ASP:HB2	1.98	0.63
1:D:229[B]:VAL:HG13	1:D:252[B]:ILE:CD1	2.29	0.62
1:D:425[A]:LYS:NZ	8:D:946:HOH:O	2.23	0.62
1:B:77[B]:ARG:HH11	1:C:117[B]:MET:HE1	1.64	0.62
1:A:350:GLU:OE1	1:A:386[B]:ILE:HG23	2.00	0.61
1:A:77[B]:ARG:HD3	8:A:784[B]:HOH:O	2.00	0.61
1:C:224:LYS:HE2	8:C:1116[B]:HOH:O	2.00	0.61
1:A:347:ALA:HB2	1:A:386[B]:ILE:HG21	1.84	0.60
1:A:450[B]:TYR:CE1	8:A:729:HOH:O	2.27	0.60
1:C:93[B]:LEU:CD1	8:C:888:HOH:O	2.48	0.60
1:C:1:MET:SD	1:C:3:LEU:HD12	2.42	0.60
1:A:347:ALA:CB	1:A:386[B]:ILE:HG21	2.32	0.59
1:A:124:ASP:HB2	8:C:1054:HOH:O	2.01	0.59
1:A:117[B]:MET:CE	1:D:77[B]:ARG:NH1	2.66	0.59
1:A:129:GLU:CG	1:A:142[B]:ILE:HD12	2.33	0.58
1:D:88:GLU:HG2	8:D:1242:HOH:O	2.02	0.58
1:B:409[A]:GLN:NE2	8:B:1012:HOH:O	2.35	0.58
3:D:502:PGE:H3	8:D:1085[B]:HOH:O	2.03	0.57
1:B:351:GLY:HA2	8:B:954:HOH:O	2.04	0.57
1:D:450[A]:TYR:CE2	8:D:1252:HOH:O	2.27	0.56
1:B:450[B]:TYR:CE2	8:B:951:HOH:O	2.21	0.56
1:D:347:ALA:CA	1:D:386[B]:ILE:HG21	2.35	0.56
1:A:450[B]:TYR:C	1:A:450[B]:TYR:CD1	2.78	0.56
8:B:1167:HOH:O	1:D:124:ASP:HB2	2.05	0.56
1:B:289[B]:CME:SG	1:B:418:LEU:HD21	2.45	0.56
1:C:224:LYS:CE	8:C:1116[B]:HOH:O	2.54	0.56
7:C:504[B]:EDO:H11	8:C:803:HOH:O	2.06	0.56
1:B:144[B]:LYS:HE2	1:B:474[B]:GLU:OE2	2.05	0.56
1:B:347:ALA:HB2	1:B:386[B]:ILE:HG21	1.87	0.55
1:D:436:LYS:NZ	8:D:1223:HOH:O	2.25	0.55
1:A:126[A]:ASP:CB	8:A:1277[A]:HOH:O	2.45	0.55
1:B:307[B]:GLN:HE21	1:B:311[B]:ASP:CG	2.10	0.55
7:C:504[B]:EDO:C1	8:C:803:HOH:O	2.55	0.55
1:D:429:LYS:NZ	8:D:1244[A]:HOH:O	2.39	0.54
1:C:1:MET:HG2	1:C:3:LEU:H	1.72	0.54
1:C:449:PRO:HB2	1:D:483[A]:LEU:CD2	2.38	0.54
1:A:339:LYS:HD2	8:A:1119:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241[B]:ILE:HD13	8:A:918:HOH:O	2.07	0.53
1:D:409[A]:GLN:HG2	8:D:876:HOH:O	2.07	0.53
1:D:409[A]:GLN:HG3	8:D:831:HOH:O	2.08	0.53
1:A:126[A]:ASP:CG	8:A:1277[A]:HOH:O	2.46	0.53
1:D:266:ASP:OD1	1:D:298[B]:GLN:OE1	2.27	0.52
1:C:347:ALA:CA	1:C:386[B]:ILE:HG21	2.40	0.52
7:C:504[B]:EDO:C2	8:C:951:HOH:O	2.58	0.52
1:A:409[A]:GLN:HG3	8:A:803:HOH:O	2.09	0.51
1:B:409[A]:GLN:HG3	8:B:738:HOH:O	2.11	0.51
1:A:244[A]:ASN:ND2	8:A:918:HOH:O	2.44	0.51
1:D:347:ALA:HA	1:D:386[B]:ILE:HG21	1.92	0.51
1:B:241[B]:ILE:HD13	8:B:1218:HOH:O	2.11	0.51
1:B:347:ALA:CA	1:B:386[B]:ILE:HG21	2.41	0.51
1:C:147[B]:VAL:HG13	1:C:477:LEU:N	2.26	0.51
1:C:289[A]:CME:CZ	8:C:1261[A]:HOH:O	2.56	0.50
1:C:409[A]:GLN:HG3	8:C:789:HOH:O	2.11	0.50
1:C:347:ALA:CB	1:C:386[B]:ILE:HG21	2.40	0.50
1:B:132:ASP:O	8:B:1167:HOH:O	2.20	0.50
1:B:351:GLY:CA	8:B:954:HOH:O	2.57	0.50
1:B:289[A]:CME:HZ2	4:B:504:PEG:C4	2.42	0.49
1:D:111[A]:ASP:OD2	1:D:450[A]:TYR:OH	2.30	0.49
1:A:346:VAL:O	1:A:350:GLU:HG3	2.13	0.49
1:B:150[B]:VAL:HG12	1:B:228[B]:LEU:HB3	1.94	0.49
8:A:1207:HOH:O	1:B:431:GLN:HG2	2.12	0.49
1:A:405:GLN:HG3	8:A:945:HOH:O	2.13	0.48
1:A:296:LEU:HD23	1:A:399:GLU:HB2	1.95	0.48
1:B:307[A]:GLN:HG3	8:B:1117:HOH:O	2.12	0.48
1:D:435[B]:ASN:ND2	8:D:800:HOH:O	2.43	0.48
1:C:431[B]:GLN:NE2	1:C:435[B]:ASN:OD1	2.42	0.48
1:C:270:PHE:CE1	1:C:304[B]:LYS:HE3	2.49	0.47
1:A:77[A]:ARG:HG3	1:A:117[A]:MET:SD	2.54	0.47
1:D:346:VAL:O	1:D:350:GLU:HG3	2.14	0.47
1:C:132:ASP:O	8:C:1054:HOH:O	2.21	0.47
1:C:346:VAL:O	1:C:350:GLU:HG3	2.15	0.47
1:C:296:LEU:HD23	1:C:399:GLU:HB2	1.97	0.47
1:D:289[B]:CME:HB3	8:D:1275[B]:HOH:O	2.14	0.47
1:B:255[B]:GLU:HG3	8:B:730:HOH:O	2.15	0.46
1:B:347:ALA:HA	1:B:386[B]:ILE:HG21	1.97	0.46
1:B:347:ALA:CB	1:B:386[B]:ILE:HG21	2.44	0.46
1:D:229[B]:VAL:CG1	1:D:252[B]:ILE:CD1	2.92	0.46
1:C:3:LEU:HD21	8:C:979:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:LEU:HD23	1:D:399:GLU:HB2	1.97	0.46
1:B:346:VAL:O	1:B:350:GLU:HG3	2.15	0.46
1:C:289[B]:CME:SD	8:C:1240:HOH:O	2.61	0.45
1:D:229[B]:VAL:CG1	1:D:252[B]:ILE:HD12	2.38	0.45
1:C:252[B]:ILE:HD11	1:C:254:LEU:HD21	1.99	0.45
1:A:80:ALA:HB1	1:A:117[B]:MET:HG2	1.99	0.45
1:C:304[B]:LYS:NZ	8:C:1101:HOH:O	2.28	0.45
1:D:377:ILE:HG21	1:D:386[B]:ILE:HD12	1.99	0.45
1:B:350:GLU:OE1	1:B:386[B]:ILE:HG23	2.17	0.45
1:B:471:GLU:OE1	8:B:990:HOH:O	2.21	0.45
1:C:425[B]:LYS:CE	8:C:893:HOH:O	2.64	0.45
1:A:409[A]:GLN:HG2	8:A:901:HOH:O	2.17	0.44
1:B:126[A]:ASP:CB	8:B:1246[A]:HOH:O	2.52	0.44
1:D:350:GLU:OE1	1:D:386[B]:ILE:HG23	2.17	0.44
1:A:362:ASP:N	8:A:1006:HOH:O	2.41	0.44
1:B:296:LEU:HD23	1:B:399:GLU:HB2	1.99	0.44
1:C:229[B]:VAL:HG13	1:C:252[B]:ILE:CD1	2.45	0.44
1:B:77[B]:ARG:HG3	1:B:117:MET:SD	2.58	0.44
1:D:231:PHE:CD1	1:D:241:ILE:CD1	3.00	0.43
1:D:339:LYS:HD2	8:D:1092:HOH:O	2.18	0.43
1:A:431[B]:GLN:NE2	1:A:435[B]:ASN:OD1	2.51	0.43
1:A:270:PHE:CE1	1:A:304[B]:LYS:HE3	2.53	0.43
1:C:144[B]:LYS:HE2	8:C:1220:HOH:O	2.17	0.43
1:C:386[B]:ILE:HD12	1:C:387:VAL:HG23	2.01	0.43
1:A:144:LYS:NZ	8:A:884:HOH:O	2.49	0.43
1:B:231:PHE:CD1	1:B:241[A]:ILE:CD1	3.02	0.42
1:B:77[B]:ARG:HD2	1:C:117[B]:MET:HE1	2.00	0.42
1:A:449:PRO:HB2	1:B:483[B]:LEU:HD13	2.00	0.42
1:B:144[B]:LYS:HE3	1:B:477:LEU:HB3	2.01	0.42
1:C:409[A]:GLN:HG2	8:C:873:HOH:O	2.18	0.42
1:B:270:PHE:CE1	1:B:304[B]:LYS:HE3	2.55	0.42
1:B:483[B]:LEU:HD23	1:B:483[B]:LEU:C	2.39	0.42
1:D:144[A]:LYS:HE2	8:D:1269:HOH:O	2.20	0.42
1:B:74:LYS:HE2	8:B:795:HOH:O	2.20	0.42
1:D:447:PHE:O	1:D:448:HIS:HB2	2.20	0.42
1:B:16:GLU:HG3	8:B:930:HOH:O	2.19	0.41
1:C:447:PHE:O	1:C:448:HIS:HB2	2.19	0.41
1:D:111[B]:ASP:OD1	8:D:987:HOH:O	2.21	0.41
1:A:252[B]:ILE:HD11	1:A:254:LEU:HD21	2.03	0.41
1:B:350:GLU:HG3	8:B:875:HOH:O	2.20	0.41
1:B:447:PHE:O	1:B:448:HIS:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:504:PEG:C2	8:A:1235:HOH:O	2.61	0.41
1:C:77[A]:ARG:HG3	1:C:117[A]:MET:SD	2.61	0.41
1:D:492:ASN:OD1	1:D:496:LYS:CE	2.69	0.41
1:B:307[B]:GLN:HG2	8:B:1117:HOH:O	2.20	0.41
1:D:252[B]:ILE:HD11	1:D:254:LEU:HD21	2.03	0.41
3:C:502:PGE:H42	8:C:1208:HOH:O	2.20	0.40
1:B:144[B]:LYS:NZ	1:B:474[B]:GLU:OE2	2.52	0.40
1:B:144[B]:LYS:CE	1:B:474[B]:GLU:OE2	2.69	0.40
1:A:307:GLN:NE2	1:A:311:ASP:OD1	2.49	0.40

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	528/520 (102%)	519 (98%)	8 (2%)	1 (0%)	47	28
1	B	526/520 (101%)	517 (98%)	8 (2%)	1 (0%)	47	28
1	C	530/520 (102%)	521 (98%)	8 (2%)	1 (0%)	47	28
1	D	519/520 (100%)	509 (98%)	9 (2%)	1 (0%)	47	28
All	All	2103/2080 (101%)	2066 (98%)	33 (2%)	4 (0%)	47	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	HIS
1	B	448	HIS
1	C	448	HIS
1	D	448	HIS

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	443/431 (103%)	436 (98%)	7 (2%)	62	41
1	B	441/431 (102%)	431 (98%)	10 (2%)	50	25
1	C	446/431 (104%)	440 (99%)	6 (1%)	69	50
1	D	435/431 (101%)	430 (99%)	5 (1%)	73	57
All	All	1765/1724 (102%)	1737 (98%)	28 (2%)	76	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252[A]	ILE
1	A	252[B]	ILE
1	A	255[A]	GLU
1	A	255[B]	GLU
1	A	284	HIS
1	A	380[A]	CYS
1	A	380[B]	CYS
1	B	77[A]	ARG
1	B	77[B]	ARG
1	B	129	GLU
1	B	252[A]	ILE
1	B	252[B]	ILE
1	B	255[A]	GLU
1	B	255[B]	GLU
1	B	284	HIS
1	B	380[A]	CYS
1	B	380[B]	CYS
1	C	84	LYS
1	C	252[A]	ILE
1	C	252[B]	ILE
1	C	284	HIS
1	C	380[A]	CYS
1	C	380[B]	CYS
1	D	252[A]	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	252[B]	ILE
1	D	284	HIS
1	D	380[A]	CYS
1	D	380[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	B	289[B]	1	8,9,10	0.98	0	5,9,11	2.09	1 (20%)
1	CME	B	289[A]	1	8,9,10	0.75	0	5,9,11	1.79	1 (20%)
1	CME	C	289[A]	1	8,9,10	0.90	0	5,9,11	1.76	2 (40%)
1	CME	A	289[B]	1	8,9,10	0.96	0	5,9,11	4.50	3 (60%)
1	CME	D	289[B]	1	8,9,10	0.82	0	5,9,11	2.89	1 (20%)
1	CME	C	289[B]	1	8,9,10	0.86	0	5,9,11	1.96	1 (20%)
1	CME	D	289[A]	1	8,9,10	0.81	0	5,9,11	1.79	1 (20%)
1	CME	A	289[A]	1	8,9,10	0.72	0	5,9,11	1.96	1 (20%)

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
1	CME	B	289[B]	1	-	1/5/8/10	-
1	CME	B	289[A]	1	-	1/5/8/10	-
1	CME	C	289[A]	1	-	3/5/8/10	-
1	CME	A	289[B]	1	-	0/5/8/10	-
1	CME	D	289[B]	1	-	2/5/8/10	-
1	CME	C	289[B]	1	-	2/5/8/10	-
1	CME	D	289[A]	1	-	2/5/8/10	-
1	CME	A	289[A]	1	-	1/5/8/10	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289[B]	CME	CB-SG-SD	9.44	128.28	103.82
1	D	289[B]	CME	CB-SG-SD	-6.19	87.78	103.82
1	A	289[A]	CME	CB-SG-SD	-4.21	92.92	103.82
1	B	289[B]	CME	CB-SG-SD	3.83	113.74	103.82
1	C	289[B]	CME	CB-SG-SD	3.82	113.73	103.82
1	B	289[A]	CME	CB-SG-SD	-3.71	94.20	103.82
1	D	289[A]	CME	CB-SG-SD	3.52	112.94	103.82
1	C	289[A]	CME	CA-CB-SG	-3.10	101.32	114.55
1	A	289[B]	CME	CZ-CE-SD	-2.60	104.35	113.37
1	A	289[B]	CME	CA-CB-SG	2.26	124.22	114.55
1	C	289[A]	CME	CE-SD-SG	-2.07	93.92	103.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	289[A]	CME	SD-CE-CZ-OH
1	C	289[B]	CME	CE-SD-SG-CB
1	D	289[A]	CME	CE-SD-SG-CB
1	C	289[A]	CME	CE-SD-SG-CB
1	C	289[A]	CME	CA-CB-SG-SD
1	A	289[A]	CME	SD-CE-CZ-OH
1	D	289[B]	CME	SD-CE-CZ-OH
1	C	289[A]	CME	SD-CE-CZ-OH
1	C	289[B]	CME	SD-CE-CZ-OH
1	D	289[A]	CME	SD-CE-CZ-OH
1	D	289[B]	CME	CE-SD-SG-CB
1	B	289[B]	CME	CZ-CE-SD-SG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	289[B]	CME	1	0
1	B	289[A]	CME	1	0
1	C	289[A]	CME	2	0
1	D	289[B]	CME	1	0
1	C	289[B]	CME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	PEG	A	505	-	6,6,6	0.46	0	5,5,5	0.18	0
3	PGE	D	502	-	9,9,9	0.52	0	8,8,8	0.56	0
4	PEG	A	504	-	6,6,6	0.59	0	5,5,5	0.52	0
4	PEG	A	506	-	6,6,6	0.43	0	5,5,5	0.24	0
5	TRS	B	505	-	7,7,7	0.29	0	9,9,9	0.45	0
3	PGE	A	502	-	9,9,9	0.48	0	8,8,8	0.51	0
6	PG4	C	503	-	12,12,12	0.46	0	11,11,11	0.56	0
3	PGE	C	502	-	9,9,9	0.57	0	8,8,8	0.31	0
4	PEG	B	504	-	6,6,6	0.39	0	5,5,5	0.18	0
5	TRS	A	507	-	7,7,7	0.32	0	9,9,9	0.33	0
3	PGE	B	502	-	9,9,9	0.42	0	8,8,8	0.25	0
7	EDO	C	504[B]	-	3,3,3	0.53	0	2,2,2	0.09	0
4	PEG	D	503	-	6,6,6	0.41	0	5,5,5	0.69	0
4	PEG	B	503	-	6,6,6	0.45	0	5,5,5	0.36	0
3	PGE	A	503	-	9,9,9	0.52	0	8,8,8	0.16	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
4	PEG	A	505	-	-	2/4/4/4	-
3	PGE	D	502	-	-	3/7/7/7	-
4	PEG	A	504	-	-	1/4/4/4	-
4	PEG	A	506	-	-	2/4/4/4	-
5	TRS	B	505	-	-	2/9/9/9	-
3	PGE	A	502	-	-	4/7/7/7	-
6	PG4	C	503	-	-	4/10/10/10	-
3	PGE	C	502	-	-	5/7/7/7	-
4	PEG	B	504	-	-	3/4/4/4	-
5	TRS	A	507	-	-	3/9/9/9	-
3	PGE	B	502	-	-	4/7/7/7	-
7	EDO	C	504[B]	-	-	0/1/1/1	-
4	PEG	D	503	-	-	1/4/4/4	-
4	PEG	B	503	-	-	3/4/4/4	-
3	PGE	A	503	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	TRS	C2-C-C1-O1
5	A	507	TRS	C3-C-C1-O1
5	A	507	TRS	N-C-C1-O1
5	B	505	TRS	N-C-C3-O3
3	A	502	PGE	C6-C5-O3-C4
6	C	503	PG4	O2-C3-C4-O3
3	C	502	PGE	O3-C5-C6-O4
4	A	506	PEG	O2-C3-C4-O4
3	C	502	PGE	O2-C3-C4-O3
3	B	502	PGE	O3-C5-C6-O4
4	A	504	PEG	O2-C3-C4-O4
6	C	503	PG4	O1-C1-C2-O2
3	B	502	PGE	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	503	PG4	O4-C7-C8-O5
5	B	505	TRS	C2-C-C3-O3
3	A	502	PGE	O3-C5-C6-O4
3	C	502	PGE	O1-C1-C2-O2
4	A	505	PEG	O1-C1-C2-O2
4	B	504	PEG	O1-C1-C2-O2
4	D	503	PEG	O1-C1-C2-O2
4	B	504	PEG	O2-C3-C4-O4
3	A	502	PGE	C4-C3-O2-C2
3	B	502	PGE	C6-C5-O3-C4
3	C	502	PGE	C6-C5-O3-C4
3	D	502	PGE	C1-C2-O2-C3
3	A	502	PGE	C3-C4-O3-C5
4	B	504	PEG	C4-C3-O2-C2
4	B	503	PEG	C4-C3-O2-C2
4	B	503	PEG	O2-C3-C4-O4
4	B	503	PEG	O1-C1-C2-O2
6	C	503	PG4	C1-C2-O2-C3
4	A	505	PEG	C4-C3-O2-C2
4	A	506	PEG	O1-C1-C2-O2
3	B	502	PGE	C3-C4-O3-C5
3	D	502	PGE	C3-C4-O3-C5
3	A	503	PGE	C4-C3-O2-C2
3	D	502	PGE	O3-C5-C6-O4
3	C	502	PGE	C3-C4-O3-C5

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	PGE	1	0
4	A	504	PEG	2	0
3	C	502	PGE	1	0
4	B	504	PEG	1	0
7	C	504[B]	EDO	3	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

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, 95^{th} 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	496/520 (95%)	-0.49	9 (1%) 68 71	8, 14, 29, 69	0
1	B	496/520 (95%)	-0.43	16 (3%) 47 48	8, 15, 32, 71	0
1	C	495/520 (95%)	-0.53	7 (1%) 75 79	8, 15, 28, 100	0
1	D	494/520 (95%)	-0.47	7 (1%) 75 79	8, 16, 30, 84	0
All	All	1981/2080 (95%)	-0.48	39 (1%) 65 67	8, 15, 30, 100	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	6.9
1	D	2	GLU	5.7
1	A	3	LEU	5.6
1	C	2	GLU	5.4
1	B	3	LEU	5.3
1	C	3	LEU	4.7
1	B	214	SER	3.8
1	C	214	SER	3.5
1	B	213	GLY	3.4
1	A	2	GLU	3.4
1	A	214	SER	3.2
1	A	1	MET	3.2
1	C	1	MET	3.2
1	C	362	ASP	3.2
1	A	0	ALA	3.1
1	B	362	ASP	3.0
1	B	2	GLU	2.9
1	D	362	ASP	2.8
1	D	364	ASP	2.8
1	B	1	MET	2.7
1	D	349	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	343	TYR	2.6
1	B	351	GLY	2.6
1	B	364	ASP	2.6
1	B	368	ASP	2.6
1	D	367	LYS	2.5
1	D	5	LYS	2.5
1	A	212	ALA	2.4
1	B	0	ALA	2.4
1	C	364	ASP	2.4
1	A	364	ASP	2.4
1	C	213	GLY	2.4
1	B	496	LYS	2.3
1	B	367	LYS	2.3
1	A	215[A]	GLU	2.3
1	B	345	ASP	2.2
1	B	212	ALA	2.1
1	A	362	ASP	2.0
1	B	5	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
1	CME	A	289[A]	10/11	0.89	0.15	18,21,34,34	10
1	CME	A	289[B]	10/11	0.89	0.15	18,23,36,37	10
1	CME	B	289[A]	10/11	0.91	0.16	18,22,34,36	10
1	CME	B	289[B]	10/11	0.91	0.16	19,25,38,40	10
1	CME	D	289[A]	10/11	0.91	0.15	19,24,47,48	10
1	CME	D	289[B]	10/11	0.91	0.15	18,20,27,31	10
1	CME	C	289[A]	10/11	0.94	0.12	15,19,27,34	10
1	CME	C	289[B]	10/11	0.94	0.12	16,21,40,41	10

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
4	PEG	B	504	7/7	0.74	0.14	49,53,59,60	0
4	PEG	A	504	7/7	0.77	0.16	41,42,51,54	0
4	PEG	A	505	7/7	0.80	0.16	48,56,61,61	0
3	PGE	C	502	10/10	0.80	0.14	42,48,56,56	0
4	PEG	D	503	7/7	0.80	0.15	40,48,54,54	0
3	PGE	A	503	10/10	0.82	0.25	40,47,55,59	0
4	PEG	A	506	7/7	0.82	0.22	48,53,62,73	0
4	PEG	B	503	7/7	0.86	0.18	47,49,55,57	0
5	TRS	B	505	8/8	0.86	0.27	42,64,74,86	0
6	PG4	C	503	13/13	0.88	0.18	31,42,55,60	0
3	PGE	B	502	10/10	0.89	0.15	38,44,46,55	0
3	PGE	D	502	10/10	0.89	0.11	45,48,55,57	0
5	TRS	A	507	8/8	0.90	0.20	41,50,53,59	0
7	EDO	C	504[B]	4/4	0.92	0.14	20,21,22,22	4
3	PGE	A	502	10/10	0.93	0.12	34,36,48,50	0
2	NA	D	501	1/1	0.99	0.04	15,15,15,15	0
2	NA	B	501	1/1	0.99	0.04	10,10,10,10	0
2	NA	A	501	1/1	1.00	0.03	11,11,11,11	0
2	NA	C	501	1/1	1.00	0.02	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.