Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:49 PM GMT

PDB ID	:	4MPY
Title	:	1.85 Angstrom resolution crystal structure of betaine aldehyde dehydrogenase (betB) from Staphylococcus aureus (IDP00699) in complex with NAD+
Authors	:	Halavaty, A.S.; Minasov, G.; Shuvalova, L.; Winsor, J.; Peterson, S.N.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-09-14
Resolution	:	1.85 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
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 (1)) were used in the production of this report:

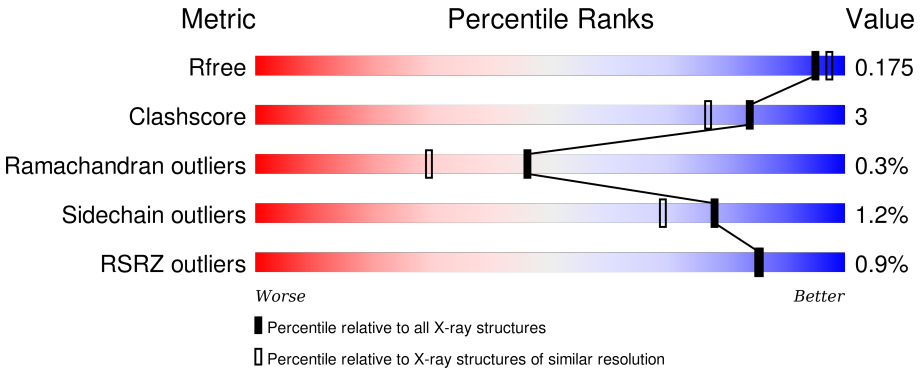
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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.

Mol	Chain	Length	Quality of chain
1	A	520	2% 91% 5% ·
1	B	520	% 91% 5% ·
1	C	520	% 90% 7% ·
1	D	520	% 89% 6% ·
1	E	520	89% 7% ·

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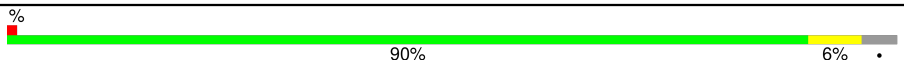
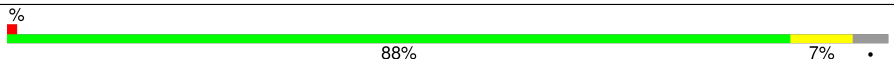
Mol	Chain	Length	Quality of chain
1	F	520	
1	G	520	
1	H	520	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	G	501	-	-	-	X
2	NAD	H	501	-	-	-	X
3	NA	F	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37293 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	500	Total	C	N	O	S	0	12	0
			3976	2503	671	785	17			
1	B	500	Total	C	N	O	S	0	10	0
			3966	2493	673	781	19			
1	C	503	Total	C	N	O	S	0	22	0
			4087	2573	687	807	20			
1	D	498	Total	C	N	O	S	0	13	0
			3969	2498	671	784	16			
1	E	501	Total	C	N	O	S	0	20	0
			4055	2552	682	801	20			
1	F	498	Total	C	N	O	S	0	21	0
			4035	2539	683	793	20			
1	G	503	Total	C	N	O	S	0	16	0
			4046	2545	687	792	22			
1	H	500	Total	C	N	O	S	0	22	0
			4066	2552	694	800	20			

There are 192 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
E	-23	MET	-	EXPRESSION TAG	UNP Q5HCU0

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

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

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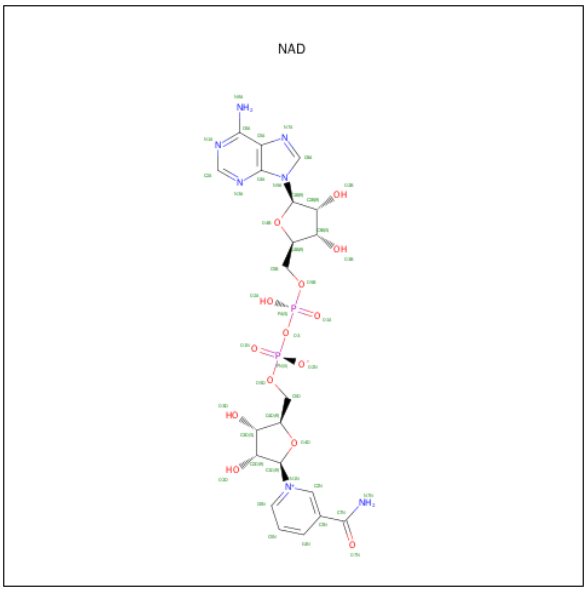
Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	GLY	-	EXPRESSION TAG	UNP Q5HCU0
H	-9	THR	-	EXPRESSION TAG	UNP Q5HCU0
H	-8	GLU	-	EXPRESSION TAG	UNP Q5HCU0
H	-7	ASN	-	EXPRESSION TAG	UNP Q5HCU0
H	-6	LEU	-	EXPRESSION TAG	UNP Q5HCU0
H	-5	TYR	-	EXPRESSION TAG	UNP Q5HCU0
H	-4	PHE	-	EXPRESSION TAG	UNP Q5HCU0
H	-3	GLN	-	EXPRESSION TAG	UNP Q5HCU0
H	-2	SER	-	EXPRESSION TAG	UNP Q5HCU0
H	-1	ASN	-	EXPRESSION TAG	UNP Q5HCU0
H	0	ALA	-	EXPRESSION TAG	UNP Q5HCU0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		
3	E	4	Total	Na	0	0
			4	4		
3	H	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	A	2	Total	Na	0	0
			2	2		
3	F	3	Total	Na	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	458	Total	O	0	14
			468	468		
4	B	501	Total	O	0	18
			516	516		
4	C	597	Total	O	0	32
			620	620		
4	D	577	Total	O	0	28
			599	599		
4	E	641	Total	O	0	32
			665	665		
4	F	646	Total	O	0	22
			667	667		

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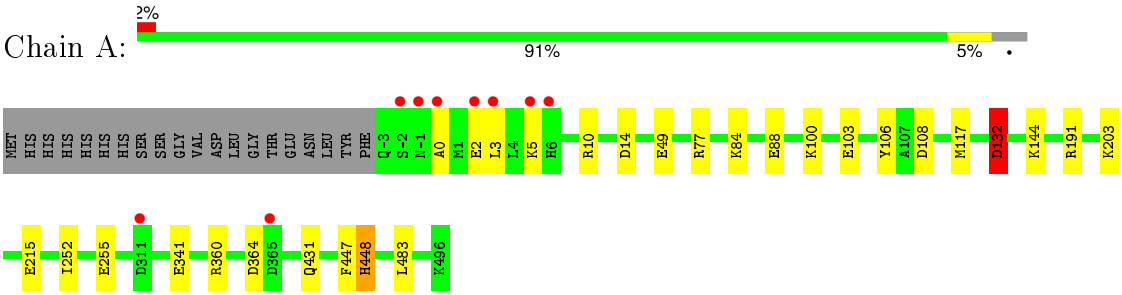
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	560	Total O 571 571	0	14
4	H	594	Total O 616 616	0	30

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.

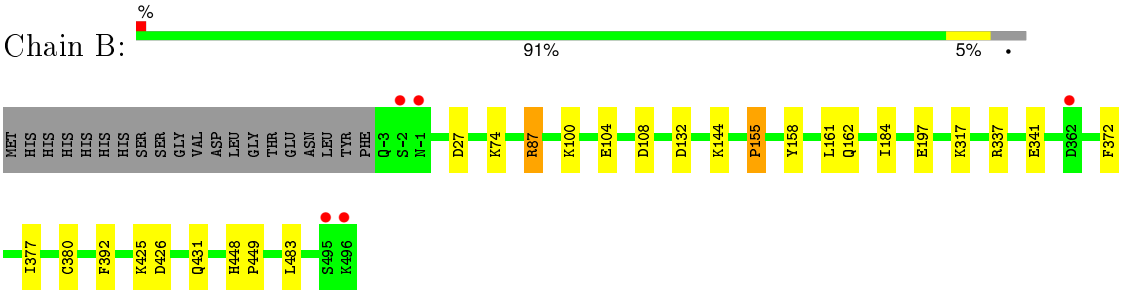
- Molecule 1: Betaine aldehyde dehydrogenase

Chain A:



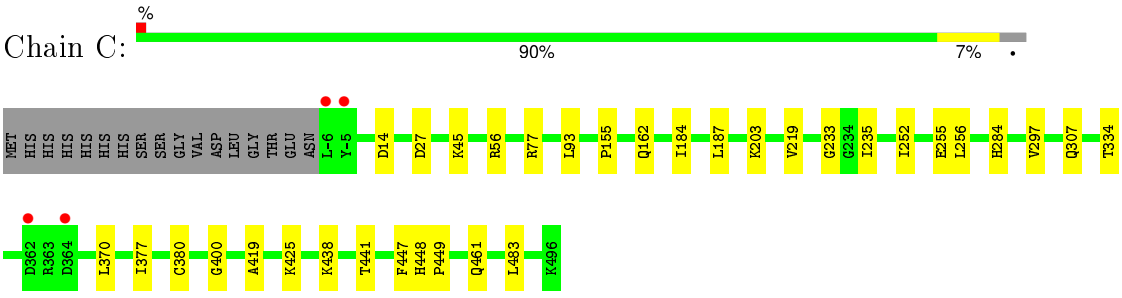
- Molecule 1: Betaine aldehyde dehydrogenase

Chain B:



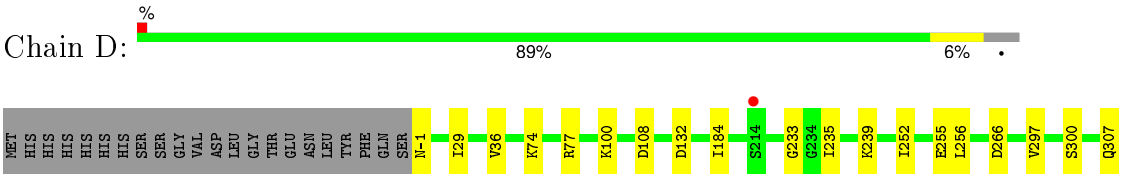
- Molecule 1: Betaine aldehyde dehydrogenase

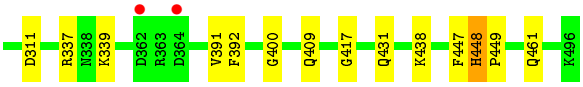
Chain C:



- Molecule 1: Betaine aldehyde dehydrogenase

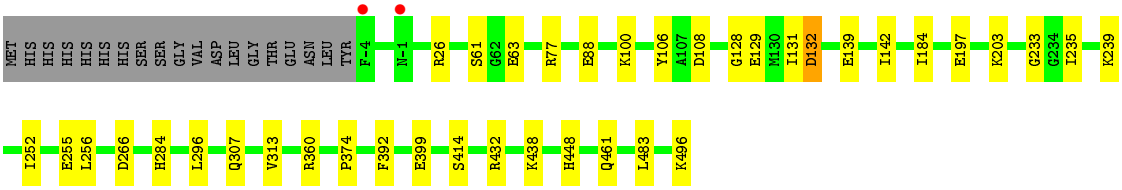
Chain D:





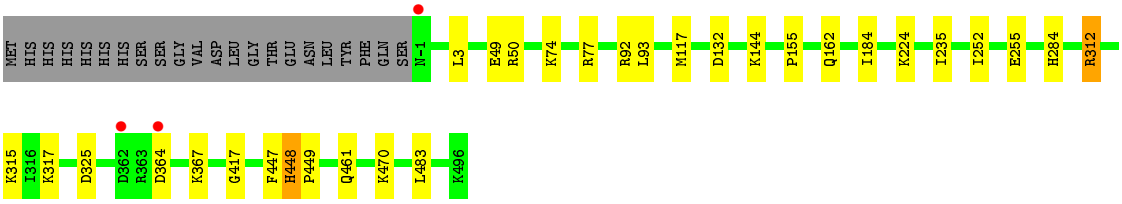
• Molecule 1: Betaine aldehyde dehydrogenase

Chain E:



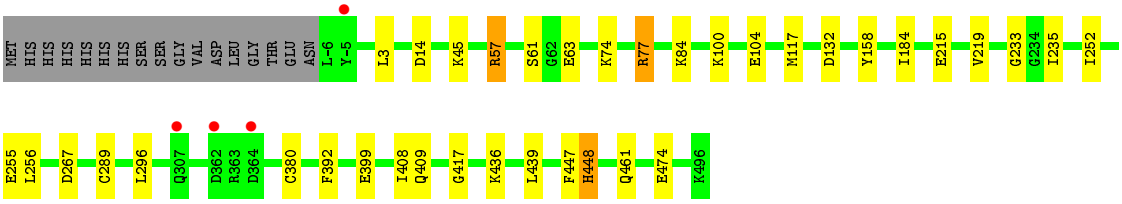
• Molecule 1: Betaine aldehyde dehydrogenase

Chain F:



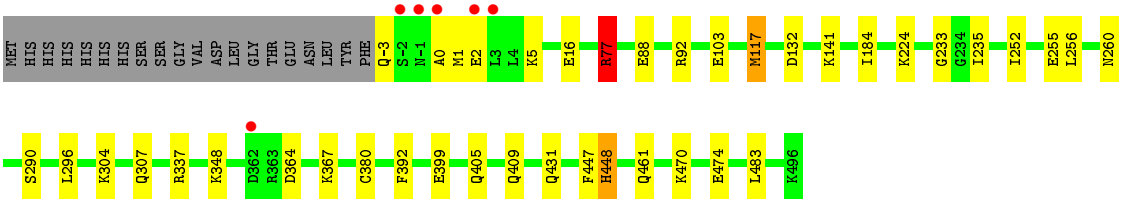
• Molecule 1: Betaine aldehyde dehydrogenase

Chain G:



• Molecule 1: Betaine aldehyde dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.87Å 159.15Å 122.99Å 90.00° 94.79° 90.00°	Depositor
Resolution (Å)	24.98 – 1.85 24.98 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.98-1.85) 99.8 (24.98-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.126 , 0.167 0.140 , 0.175	Depositor DCC
R_{free} test set	9843 reflections (3.13%)	DCC
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 324065 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	37293	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 19.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CME, NAD

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	0.58	0/4036	0.80	2/5452 (0.0%)
1	B	0.60	1/4016 (0.0%)	0.82	4/5425 (0.1%)
1	C	0.62	1/4139 (0.0%)	0.84	2/5593 (0.0%)
1	D	0.63	1/4029 (0.0%)	0.82	1/5442 (0.0%)
1	E	0.65	1/4106 (0.0%)	0.83	3/5546 (0.1%)
1	F	0.64	1/4085 (0.0%)	0.84	2/5515 (0.0%)
1	G	0.61	1/4098 (0.0%)	0.83	5/5532 (0.1%)
1	H	0.62	1/4116 (0.0%)	0.81	2/5556 (0.0%)
All	All	0.62	7/32625 (0.0%)	0.82	21/44061 (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	G	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	184	ILE	C-O	5.84	1.34	1.23
1	D	184	ILE	C-O	5.78	1.34	1.23
1	G	184	ILE	C-O	5.77	1.34	1.23
1	H	184	ILE	C-O	5.77	1.34	1.23
1	E	184	ILE	C-O	5.71	1.34	1.23
1	F	184	ILE	C-O	5.22	1.33	1.23
1	B	184	ILE	C-O	5.12	1.33	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	432	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	G	57[A]	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	G	57[B]	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	F	312	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	F	50	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	E	360	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	337	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	D	337	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	H	77[A]	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	H	77[B]	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	27	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	57[A]	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	57[B]	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	56	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	191	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	132	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	G	267	ASP	CB-CG-OD1	5.25	123.02	118.30
1	B	337	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	27	ASP	CB-CG-OD1	5.13	122.91	118.30
1	E	432	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	426	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	77[A]	ARG	Sidechain

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	3976	0	3914	20	0
1	B	3966	0	3902	22	0
1	C	4087	0	4010	20	0
1	D	3969	0	3907	23	0
1	E	4055	0	3980	34	0
1	F	4035	0	3974	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4046	0	3980	31	0
1	H	4066	0	3998	43	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	468	0	0	13	0
4	B	516	0	0	6	0
4	C	620	0	0	8	0
4	D	599	0	0	9	0
4	E	665	0	0	5	0
4	F	667	0	0	11	0
4	G	571	0	0	11	0
4	H	616	0	0	19	0
All	All	37293	0	31873	197	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 3.

All (197) 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:D:235[A]:ILE:HD11	1:D:461:GLN:OE1	1.46	1.14
1:H:337[B]:ARG:HH11	1:H:337[B]:ARG:HG2	1.20	1.00
1:C:235[B]:ILE:HD11	1:C:461:GLN:OE1	1.63	0.98
1:H:307:GLN:HG2	4:H:685:HOH:O	1.68	0.90
1:E:235[B]:ILE:HD11	1:E:461:GLN:OE1	1.76	0.86
1:H:337[B]:ARG:CG	1:H:337[B]:ARG:HH11	1.91	0.83
1:F:144:LYS:HE2	4:F:969:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LYS:HG3	4:B:1057:HOH:O	1.79	0.81
1:E:77:ARG:HD3	1:G:77[B]:ARG:HH21	1.43	0.81
1:G:77[B]:ARG:CZ	4:G:603:HOH:O	2.30	0.78
1:H:431:GLN:HG3	4:H:1056:HOH:O	1.86	0.76
1:E:77:ARG:HD3	1:G:77[B]:ARG:NH2	2.00	0.75
1:A:10:ARG:NH1	4:A:941:HOH:O	2.20	0.75
1:H:337[B]:ARG:NH1	1:H:337[B]:ARG:HG2	1.95	0.73
1:D:307[A]:GLN:NE2	1:D:311[A]:ASP:OD1	2.21	0.72
1:C:334[B]:THR:CG2	4:C:1018:HOH:O	2.37	0.72
1:H:235[B]:ILE:HD11	1:H:461:GLN:OE1	1.90	0.72
1:F:49[A]:GLU:CD	4:F:819:HOH:O	2.28	0.71
1:B:197:GLU:OE2	1:H:304:LYS:HE3	1.93	0.69
1:H:405[B]:GLN:O	1:H:409[B]:GLN:HG3	1.92	0.69
1:H:337[B]:ARG:NH1	4:H:1082:HOH:O	2.25	0.69
1:H:117[A]:MET:HA	1:H:117[A]:MET:CE	2.23	0.68
1:F:117[B]:MET:CE	1:H:77[B]:ARG:NH1	2.57	0.67
1:F:77:ARG:HD3	1:H:77[B]:ARG:HD3	1.77	0.66
1:G:235:ILE:HD11	1:G:461:GLN:OE1	1.94	0.66
1:C:334[B]:THR:HG21	4:C:1018:HOH:O	1.96	0.64
1:H:348:LYS:CE	4:H:945[A]:HOH:O	2.45	0.63
1:G:77[A]:ARG:NH2	4:G:966:HOH:O	2.30	0.63
1:A:2:GLU:O	1:A:5:LYS:HG2	1.99	0.63
1:G:77[B]:ARG:NH2	4:G:603:HOH:O	2.31	0.63
1:C:334[B]:THR:HG22	4:C:1018:HOH:O	1.98	0.62
4:C:1188[A]:HOH:O	1:D:431:GLN:HG2	1.99	0.62
1:F:483[A]:LEU:C	1:F:483[A]:LEU:HD23	2.20	0.62
4:A:960[B]:HOH:O	1:B:431[B]:GLN:NE2	2.33	0.61
1:D:235[A]:ILE:CD1	1:D:461:GLN:OE1	2.36	0.61
1:H:16:GLU:HG3	4:H:1071:HOH:O	2.01	0.61
1:E:496:LYS:HD3	1:F:315[A]:LYS:HD3	1.83	0.61
1:E:77:ARG:HG2	1:G:77[B]:ARG:HH22	1.66	0.61
1:A:144:LYS:HD2	4:A:1011:HOH:O	2.00	0.61
1:H:405[B]:GLN:HG3	4:H:977[B]:HOH:O	2.00	0.60
1:B:74:LYS:HE2	4:D:807:HOH:O	2.01	0.60
1:A:103[B]:GLU:HG3	4:A:726:HOH:O	2.01	0.59
1:E:100[A]:LYS:HE3	1:E:108:ASP:OD2	2.02	0.59
1:G:408:ILE:HD13	1:G:436:LYS:HD2	1.84	0.58
1:E:77:ARG:HD3	1:G:77[A]:ARG:HD3	1.85	0.58
1:E:496:LYS:HD2	1:F:317[A]:LYS:HZ1	1.68	0.58
1:H:296:LEU:HD23	1:H:399:GLU:HB2	1.86	0.58
1:E:132:ASP:HB2	4:E:1183:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:483[A]:LEU:C	1:H:483[A]:LEU:HD23	2.25	0.57
1:B:425:LYS:NZ	4:B:1006:HOH:O	2.36	0.56
1:E:139:GLU:OE1	1:H:141:LYS:NZ	2.33	0.56
1:C:307:GLN:HG3	4:C:1110[A]:HOH:O	2.05	0.56
1:D:409:GLN:HG2	4:D:1158:HOH:O	2.05	0.56
1:E:77:ARG:CD	1:G:77[B]:ARG:NH2	2.69	0.55
1:E:307:GLN:CD	4:E:814:HOH:O	2.45	0.55
1:E:307:GLN:HG3	4:E:1053:HOH:O	2.06	0.55
1:G:296:LEU:HD23	1:G:399:GLU:HB2	1.89	0.55
1:G:215:GLU:HG2	4:G:1020:HOH:O	2.07	0.55
1:B:100[A]:LYS:CD	4:B:849[A]:HOH:O	2.56	0.54
1:D:-1:ASN:N	4:D:1099:HOH:O	2.40	0.54
1:H:409[B]:GLN:HG2	4:H:1124:HOH:O	2.06	0.54
1:D:74[A]:LYS:HE2	4:D:760:HOH:O	2.07	0.54
1:H:470:LYS:NZ	4:H:612:HOH:O	2.40	0.53
1:F:312:ARG:HD3	4:F:1096:HOH:O	2.09	0.53
1:F:93[B]:LEU:HD12	4:F:1066:HOH:O	2.09	0.52
1:H:103:GLU:HG2	4:H:1045:HOH:O	2.08	0.52
1:C:93[A]:LEU:HD11	1:C:187:LEU:HB3	1.92	0.52
1:G:436:LYS:HE2	4:G:999:HOH:O	2.10	0.52
1:C:45:LYS:HB2	1:C:219:VAL:HG21	1.92	0.51
1:A:431:GLN:HG2	4:A:1047:HOH:O	2.11	0.51
1:A:364:ASP:N	4:A:1001:HOH:O	2.42	0.51
1:A:341:GLU:OE2	1:A:360:ARG:NE	2.35	0.51
1:G:3:LEU:HB3	4:G:1003:HOH:O	2.10	0.51
1:G:100[A]:LYS:HG2	1:G:104:GLU:HB2	1.94	0.50
1:H:0:ALA:HB2	1:H:92:ARG:HB3	1.94	0.50
1:D:100:LYS:HE3	1:D:108:ASP:OD2	2.12	0.50
1:H:117[A]:MET:HE2	1:H:117[A]:MET:CA	2.41	0.50
1:H:103:GLU:CG	4:H:1045:HOH:O	2.59	0.50
1:H:88:GLU:HG2	4:H:774:HOH:O	2.10	0.50
1:G:14:ASP:OD2	1:G:57[B]:ARG:NH2	2.44	0.50
1:H:337[B]:ARG:NE	4:H:1194[B]:HOH:O	2.26	0.50
1:C:77[A]:ARG:HG2	1:C:77[A]:ARG:O	2.10	0.50
1:B:144:LYS:HD2	4:B:718:HOH:O	2.12	0.50
1:E:235[B]:ILE:CG1	1:E:239:LYS:HE3	2.42	0.50
1:B:87[A]:ARG:NH2	1:E:266:ASP:OD1	2.45	0.49
1:H:117[A]:MET:HE2	1:H:117[A]:MET:HA	1.92	0.49
1:G:77[A]:ARG:HG3	1:G:117[A]:MET:SD	2.52	0.49
1:E:77:ARG:CG	1:G:77[B]:ARG:NH2	2.75	0.49
1:E:235[B]:ILE:HG12	1:E:239:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:474:GLU:HG2	4:H:1125:HOH:O	2.12	0.49
1:H:364:ASP:OD1	1:H:367:LYS:HE2	2.13	0.48
1:D:307[A]:GLN:HE21	1:D:311[A]:ASP:CG	2.17	0.48
1:A:88:GLU:OE2	1:A:106:TYR:OH	2.26	0.48
1:H:224:LYS:NZ	4:H:1179:HOH:O	2.46	0.48
1:D:74[B]:LYS:CE	4:D:989:HOH:O	2.62	0.48
1:A:49[B]:GLU:HG3	4:A:772:HOH:O	2.12	0.48
1:E:296:LEU:HD23	1:E:399:GLU:HB2	1.96	0.47
1:B:377:ILE:HG22	1:B:380[A]:CYS:SG	2.54	0.47
4:A:960[B]:HOH:O	1:B:431[B]:GLN:CG	2.63	0.47
1:C:438:LYS:HE3	4:D:767:HOH:O	2.15	0.47
1:B:87[A]:ARG:NH1	1:E:266:ASP:OD2	2.48	0.47
1:E:313:VAL:HG13	1:E:374:PRO:HB2	1.96	0.47
1:B:197:GLU:OE2	1:H:304:LYS:CE	2.61	0.47
1:F:155:PRO:HG2	1:F:162[B]:GLN:OE1	2.14	0.47
1:E:197:GLU:OE2	4:E:1235:HOH:O	2.21	0.46
1:G:235:ILE:HD11	1:G:461:GLN:HB3	1.96	0.46
1:C:14:ASP:OD1	1:C:203:LYS:HG2	2.15	0.46
1:G:474:GLU:HG2	4:G:1027:HOH:O	2.14	0.46
1:A:447:PHE:O	1:A:448:HIS:HB2	2.16	0.46
4:A:960[B]:HOH:O	1:B:431[B]:GLN:HG2	2.16	0.46
1:G:74:LYS:HE2	4:G:941:HOH:O	2.16	0.45
1:C:155:PRO:HG2	1:C:162[B]:GLN:OE1	2.16	0.45
1:F:77:ARG:NH2	4:F:960:HOH:O	2.48	0.45
1:E:496:LYS:CD	1:F:317[A]:LYS:HZ1	2.29	0.45
1:G:447:PHE:O	1:G:448:HIS:HB2	2.17	0.45
1:A:483[A]:LEU:C	1:A:483[A]:LEU:HD23	2.36	0.45
1:C:77[B]:ARG:NH2	4:C:985:HOH:O	2.49	0.45
1:H:260:ASN:ND2	1:H:290:SER:HA	2.32	0.45
1:H:77[A]:ARG:NH2	4:H:842:HOH:O	2.44	0.45
1:A:84:LYS:NZ	4:A:787:HOH:O	2.50	0.45
1:F:447:PHE:O	1:F:448:HIS:HB2	2.15	0.45
1:H:233:GLY:O	1:H:256:LEU:HA	2.17	0.45
1:G:158:TYR:CD1	1:G:289[B]:CME:CZ	2.99	0.45
1:B:197:GLU:HG3	1:H:304:LYS:HE3	1.99	0.45
1:E:233:GLY:O	1:E:256:LEU:HA	2.17	0.45
1:B:74:LYS:HE3	4:B:782:HOH:O	2.17	0.45
1:B:100[B]:LYS:HE3	1:B:108:ASP:OD2	2.16	0.45
1:H:117[A]:MET:HE3	1:H:117[A]:MET:HA	1.96	0.44
1:H:2:GLU:O	1:H:5:LYS:HG2	2.17	0.44
1:G:84:LYS:NZ	4:G:921:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:GLN:HG3	4:H:1154:HOH:O	2.18	0.44
1:A:144:LYS:CD	4:A:1011:HOH:O	2.62	0.44
1:F:49[A]:GLU:CG	4:F:819:HOH:O	2.65	0.44
1:D:233:GLY:O	1:D:256:LEU:HA	2.18	0.44
1:B:341:GLU:HG2	1:B:372:PHE:HE1	1.82	0.44
1:C:483[A]:LEU:CD2	1:D:449:PRO:HB2	2.48	0.44
1:A:14:ASP:OD1	1:A:203:LYS:HG2	2.17	0.44
1:F:483[A]:LEU:CD2	1:F:483[A]:LEU:C	2.86	0.44
1:F:3:LEU:HD11	1:F:92:ARG:HB3	1.99	0.44
1:D:235[A]:ILE:CG1	1:D:239:LYS:HE3	2.48	0.43
1:C:377:ILE:HG22	1:C:380[A]:CYS:SG	2.58	0.43
1:F:317[B]:LYS:HD2	1:F:325:ASP:O	2.18	0.43
1:E:77:ARG:HG2	1:G:77[B]:ARG:NH2	2.30	0.43
1:C:334[B]:THR:HG22	1:C:370:LEU:HD21	2.00	0.43
1:E:496:LYS:O	1:F:312:ARG:NE	2.47	0.43
1:F:367[A]:LYS:HB2	1:F:367[A]:LYS:HE3	1.71	0.43
1:D:266:ASP:CG	1:D:300:SER:HB2	2.39	0.43
1:A:0:ALA:O	1:A:3:LEU:HB2	2.19	0.43
1:E:26:ARG:NH1	4:E:1057:HOH:O	2.49	0.43
1:G:45:LYS:HB2	1:G:219:VAL:HG21	2.00	0.43
1:B:100[A]:LYS:HD2	1:B:104:GLU:HB3	2.00	0.43
1:D:74[B]:LYS:HE2	4:D:989:HOH:O	2.18	0.43
1:F:470:LYS:NZ	4:H:612:HOH:O	2.49	0.43
1:G:61[B]:SER:OG	1:G:63:GLU:OE1	2.23	0.43
1:A:483[B]:LEU:CD2	1:B:449:PRO:HB2	2.49	0.43
1:F:224:LYS:NZ	4:F:1008:HOH:O	2.51	0.43
1:B:155:PRO:HG2	1:B:162[B]:GLN:OE1	2.18	0.43
1:D:297:VAL:O	1:D:400:GLY:HA2	2.19	0.43
1:D:431:GLN:NE2	4:D:1173:HOH:O	2.51	0.42
1:F:235:ILE:HD11	1:F:461:GLN:OE1	2.19	0.42
1:E:88:GLU:OE2	1:E:106:TYR:CZ	2.72	0.42
1:D:29:ILE:HD13	1:D:36:VAL:HA	2.01	0.42
1:G:77[B]:ARG:CZ	4:G:1158:HOH:O	2.68	0.42
1:G:409:GLN:NE2	4:G:1115:HOH:O	2.41	0.42
1:E:61:SER:OG	1:E:63:GLU:OE1	2.21	0.42
1:H:348:LYS:NZ	4:H:945[B]:HOH:O	2.52	0.42
1:C:233:GLY:O	1:C:256:LEU:HA	2.20	0.42
1:F:117[B]:MET:HE1	1:H:77[B]:ARG:NH1	2.34	0.42
1:D:235[A]:ILE:HG12	1:D:239:LYS:HE3	2.01	0.42
1:D:74[A]:LYS:CE	4:D:760:HOH:O	2.67	0.42
1:H:-3:GLN:O	1:H:1:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ALA:HA	1:C:441:THR:O	2.20	0.42
1:C:447:PHE:C	1:C:449:PRO:HD3	2.40	0.42
1:G:233:GLY:O	1:G:256:LEU:HA	2.20	0.42
1:H:447:PHE:O	1:H:448:HIS:HB2	2.20	0.42
1:C:297:VAL:O	1:C:400:GLY:HA2	2.21	0.41
1:A:77:ARG:HG3	1:A:117[A]:MET:SD	2.60	0.41
1:B:87[A]:ARG:NH1	4:B:889:HOH:O	2.53	0.41
1:D:447:PHE:O	1:D:448:HIS:HB2	2.20	0.41
1:E:128:GLY:HA3	1:E:142[B]:ILE:O	2.20	0.41
1:E:438:LYS:HE3	4:F:893:HOH:O	2.20	0.41
1:E:129:GLU:CG	1:E:142[A]:ILE:HD12	2.50	0.41
1:E:131:ILE:HD11	1:E:142[A]:ILE:CD1	2.51	0.41
1:F:93[B]:LEU:CD1	4:F:1066:HOH:O	2.67	0.41
1:A:132:ASP:CG	4:A:902:HOH:O	2.58	0.41
1:G:417:GLY:HA2	1:G:439:LEU:HD23	2.03	0.41
1:E:88:GLU:OE2	1:E:106:TYR:CE1	2.74	0.41
1:A:100[B]:LYS:HE3	1:A:108[B]:ASP:OD2	2.21	0.41
1:D:339:LYS:HE2	1:D:391:VAL:O	2.21	0.40
1:B:158:TYR:HB3	1:B:161:LEU:HB3	2.02	0.40
1:E:483[A]:LEU:CD2	1:F:449:PRO:HB2	2.51	0.40
1:H:431:GLN:CG	4:H:1056:HOH:O	2.59	0.40
1:C:425:LYS:HE2	4:C:1148:HOH:O	2.21	0.40
1:F:49[A]:GLU:HG3	4:F:819:HOH:O	2.20	0.40
1:F:74:LYS:HE2	4:F:970:HOH:O	2.21	0.40
1:A:215:GLU:HG2	4:A:828:HOH:O	2.22	0.40
4:C:1150:HOH:O	1:D:438[A]:LYS:HE3	2.20	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	509/520 (98%)	498 (98%)	10 (2%)	1 (0%)	52	36
1	B	506/520 (97%)	498 (98%)	6 (1%)	2 (0%)	39	22
1	C	521/520 (100%)	512 (98%)	8 (2%)	1 (0%)	52	36
1	D	508/520 (98%)	498 (98%)	8 (2%)	2 (0%)	39	22
1	E	517/520 (99%)	506 (98%)	10 (2%)	1 (0%)	52	36
1	F	515/520 (99%)	505 (98%)	8 (2%)	2 (0%)	39	22
1	G	515/520 (99%)	506 (98%)	8 (2%)	1 (0%)	52	36
1	H	518/520 (100%)	507 (98%)	10 (2%)	1 (0%)	52	36
All	All	4109/4160 (99%)	4030 (98%)	68 (2%)	11 (0%)	46	29

All (11) 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
1	E	448	HIS
1	F	448	HIS
1	G	448	HIS
1	H	448	HIS
1	B	155	PRO
1	D	417	GLY
1	F	417	GLY

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	425/431 (99%)	422 (99%)	3 (1%)	88	84
1	B	422/431 (98%)	417 (99%)	5 (1%)	78	69
1	C	437/431 (101%)	434 (99%)	3 (1%)	88	84
1	D	424/431 (98%)	419 (99%)	5 (1%)	78	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	433/431 (100%)	426 (98%)	7 (2%)	70 57
1	F	430/431 (100%)	424 (99%)	6 (1%)	74 63
1	G	431/431 (100%)	425 (99%)	6 (1%)	74 63
1	H	434/431 (101%)	424 (98%)	10 (2%)	58 41
All	All	3436/3448 (100%)	3391 (99%)	45 (1%)	78 65

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	252	ILE
1	A	255	GLU
1	B	87[A]	ARG
1	B	87[B]	ARG
1	B	132	ASP
1	B	392	PHE
1	B	483	LEU
1	C	252	ILE
1	C	255	GLU
1	C	284	HIS
1	D	77	ARG
1	D	132	ASP
1	D	252	ILE
1	D	255	GLU
1	D	392	PHE
1	E	132	ASP
1	E	203	LYS
1	E	252	ILE
1	E	255	GLU
1	E	284	HIS
1	E	392	PHE
1	E	414	SER
1	F	132	ASP
1	F	252	ILE
1	F	255	GLU
1	F	284	HIS
1	F	364[A]	ASP
1	F	364[B]	ASP
1	G	132	ASP
1	G	252	ILE
1	G	255	GLU

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Mol	Chain	Res	Type
1	G	380[A]	CYS
1	G	380[B]	CYS
1	G	392	PHE
1	H	77[A]	ARG
1	H	77[B]	ARG
1	H	117[A]	MET
1	H	117[B]	MET
1	H	132	ASP
1	H	252	ILE
1	H	255	GLU
1	H	380[A]	CYS
1	H	380[B]	CYS
1	H	392	PHE

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

Mol	Chain	Res	Type
1	H	-1	ASN
1	H	307	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)

14 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	A	289	1	8,9,10	0.68	0	6,9,11	4.55	3 (50%)
1	CME	B	289[A]	1	8,9,10	0.70	0	6,9,11	1.29	0
1	CME	B	289[B]	1	8,9,10	0.70	0	6,9,11	2.74	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CME	C	289[A]	1	8,9,10	0.65	0	6,9,11	1.72	1 (16%)
1	CME	C	289[B]	1	8,9,10	0.65	0	6,9,11	3.38	1 (16%)
1	CME	D	289	1	8,9,10	0.77	0	6,9,11	1.37	1 (16%)
1	CME	E	289[A]	1	8,9,10	0.71	0	6,9,11	1.26	0
1	CME	E	289[B]	1	8,9,10	0.71	0	6,9,11	3.59	2 (33%)
1	CME	F	289[A]	1	8,9,10	0.76	0	6,9,11	2.83	2 (33%)
1	CME	F	289[B]	1	8,9,10	0.71	0	6,9,11	1.08	0
1	CME	G	289[A]	1	8,9,10	0.76	0	6,9,11	1.64	1 (16%)
1	CME	G	289[B]	1	8,9,10	0.77	0	6,9,11	2.70	2 (33%)
1	CME	H	289[A]	1	8,9,10	0.79	0	6,9,11	1.28	1 (16%)
1	CME	H	289[B]	1	8,9,10	0.74	0	6,9,11	3.13	1 (16%)

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	A	289	1	-	0/5/8/10	0/0/0/0
1	CME	B	289[A]	1	-	0/5/8/10	0/0/0/0
1	CME	B	289[B]	1	-	0/5/8/10	0/0/0/0
1	CME	C	289[A]	1	-	0/5/8/10	0/0/0/0
1	CME	C	289[B]	1	-	0/5/8/10	0/0/0/0
1	CME	D	289	1	-	0/5/8/10	0/0/0/0
1	CME	E	289[A]	1	-	0/5/8/10	0/0/0/0
1	CME	E	289[B]	1	-	0/5/8/10	0/0/0/0
1	CME	F	289[A]	1	-	0/5/8/10	0/0/0/0
1	CME	F	289[B]	1	-	0/5/8/10	0/0/0/0
1	CME	G	289[A]	1	-	0/5/8/10	0/0/0/0
1	CME	G	289[B]	1	-	0/5/8/10	0/0/0/0
1	CME	H	289[A]	1	-	0/5/8/10	0/0/0/0
1	CME	H	289[B]	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	CME	CZ-CE-SD	-4.73	101.61	113.16
1	F	289[A]	CME	CZ-CE-SD	-2.59	106.84	113.16
1	G	289[B]	CME	CZ-CE-SD	-2.45	107.18	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	289[B]	CME	CZ-CE-SD	-2.38	107.33	113.16
1	A	289	CME	O-C-CA	-2.08	120.06	125.49
1	D	289	CME	CZ-CE-SD	-2.08	108.08	113.16
1	H	289[A]	CME	CB-SG-SD	2.30	108.43	103.95
1	C	289[A]	CME	CB-SG-SD	3.48	110.74	103.95
1	G	289[A]	CME	CB-SG-SD	3.55	110.87	103.95
1	G	289[B]	CME	CB-SG-SD	5.81	115.27	103.95
1	F	289[A]	CME	CB-SG-SD	6.07	115.77	103.95
1	B	289[B]	CME	CB-SG-SD	6.11	115.86	103.95
1	H	289[B]	CME	CB-SG-SD	7.15	117.88	103.95
1	C	289[B]	CME	CB-SG-SD	7.65	118.86	103.95
1	E	289[B]	CME	CB-SG-SD	8.13	119.80	103.95
1	A	289	CME	CB-SG-SD	9.81	123.07	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	289[B]	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 19 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	NAD	A	501	-	38,48,48	1.00	1 (2%)	47,73,73	1.91	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	B	501	-	38,48,48	0.86	2 (5%)	47,73,73	1.86	4 (8%)
2	NAD	C	501	-	38,48,48	1.04	1 (2%)	47,73,73	1.82	6 (12%)
2	NAD	D	501	-	38,48,48	1.01	2 (5%)	47,73,73	1.97	7 (14%)
2	NAD	E	501	-	38,48,48	1.03	1 (2%)	47,73,73	1.98	8 (17%)
2	NAD	F	501	-	38,48,48	0.84	1 (2%)	47,73,73	1.54	5 (10%)
2	NAD	G	501	-	38,48,48	1.09	4 (10%)	47,73,73	1.92	8 (17%)
2	NAD	H	501	-	38,48,48	1.04	2 (5%)	47,73,73	1.59	3 (6%)

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	NAD	A	501	-	-	0/22/62/62	0/5/5/5
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5
2	NAD	E	501	-	-	0/22/62/62	0/5/5/5
2	NAD	F	501	-	-	0/22/62/62	0/5/5/5
2	NAD	G	501	-	-	0/22/62/62	0/5/5/5
2	NAD	H	501	-	-	0/22/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O4D-C1D	2.05	1.43	1.41
2	D	501	NAD	C2A-N3A	2.08	1.35	1.32
2	H	501	NAD	C2A-N3A	2.14	1.36	1.32
2	G	501	NAD	C2A-N3A	2.40	1.36	1.32
2	G	501	NAD	O4D-C1D	2.45	1.44	1.41
2	B	501	NAD	O7N-C7N	2.63	1.29	1.24
2	G	501	NAD	O4B-C1B	2.71	1.44	1.41
2	F	501	NAD	O7N-C7N	3.42	1.31	1.24
2	G	501	NAD	O7N-C7N	3.57	1.31	1.24
2	C	501	NAD	O7N-C7N	4.06	1.32	1.24
2	E	501	NAD	O7N-C7N	4.11	1.32	1.24
2	H	501	NAD	O7N-C7N	4.33	1.33	1.24
2	A	501	NAD	O7N-C7N	4.54	1.33	1.24
2	D	501	NAD	O7N-C7N	4.75	1.34	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAD	N3A-C2A-N1A	-10.01	121.23	128.89
2	C	501	NAD	N3A-C2A-N1A	-9.54	121.59	128.89
2	D	501	NAD	N3A-C2A-N1A	-8.91	122.07	128.89
2	G	501	NAD	N3A-C2A-N1A	-8.64	122.28	128.89
2	A	501	NAD	N3A-C2A-N1A	-8.60	122.31	128.89
2	E	501	NAD	N3A-C2A-N1A	-8.52	122.37	128.89
2	H	501	NAD	N3A-C2A-N1A	-8.17	122.64	128.89
2	F	501	NAD	N3A-C2A-N1A	-6.58	123.86	128.89
2	G	501	NAD	C4A-C5A-N7A	-4.21	105.60	109.48
2	A	501	NAD	C4A-C5A-N7A	-4.07	105.73	109.48
2	G	501	NAD	C1B-N9A-C4A	-4.06	120.82	126.94
2	E	501	NAD	C1B-N9A-C4A	-3.72	121.32	126.94
2	D	501	NAD	O3-PA-O5B	-3.63	93.31	102.94
2	D	501	NAD	C1B-N9A-C4A	-3.60	121.51	126.94
2	C	501	NAD	C1B-N9A-C4A	-3.46	121.72	126.94
2	E	501	NAD	O7N-C7N-N7N	-3.03	118.33	122.59
2	E	501	NAD	C4A-C5A-N7A	-2.99	106.73	109.48
2	D	501	NAD	C4A-C5A-N7A	-2.62	107.07	109.48
2	G	501	NAD	O7N-C7N-N7N	-2.62	118.91	122.59
2	E	501	NAD	O3-PA-O5B	-2.59	96.07	102.94
2	F	501	NAD	C1B-N9A-C4A	-2.40	123.32	126.94
2	G	501	NAD	O3-PA-O5B	-2.33	96.76	102.94
2	A	501	NAD	C1B-N9A-C4A	-2.24	123.56	126.94
2	C	501	NAD	C4B-O4B-C1B	-2.09	107.42	109.72
2	C	501	NAD	C2D-C3D-C4D	-2.08	98.34	102.61
2	B	501	NAD	C4B-O4B-C1B	-2.04	107.47	109.72
2	H	501	NAD	C1B-N9A-C4A	-2.00	123.92	126.94
2	F	501	NAD	O4D-C1D-N1N	2.01	110.34	108.13
2	G	501	NAD	O2N-PN-O1N	2.05	123.63	112.53
2	F	501	NAD	O3D-C3D-C2D	2.14	118.80	111.83
2	D	501	NAD	O2N-PN-O1N	2.16	124.22	112.53
2	D	501	NAD	C2N-C3N-C4N	2.23	120.78	118.29
2	B	501	NAD	C2N-C3N-C4N	2.28	120.83	118.29
2	C	501	NAD	O4D-C1D-N1N	2.35	110.72	108.13
2	A	501	NAD	O4B-C1B-N9A	2.40	113.13	108.10
2	F	501	NAD	C2N-C3N-C4N	2.42	120.98	118.29
2	E	501	NAD	O4B-C1B-N9A	2.45	113.23	108.10
2	E	501	NAD	C3N-C7N-N7N	2.63	120.70	117.82
2	G	501	NAD	C3N-C7N-N7N	2.67	120.73	117.82
2	G	501	NAD	O4D-C1D-N1N	2.75	111.15	108.13
2	C	501	NAD	O2N-PN-O3	2.75	117.58	105.09
2	H	501	NAD	C3N-C7N-N7N	3.31	121.44	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAD	O4D-C1D-N1N	3.55	112.03	108.13
2	E	501	NAD	O4D-C1D-N1N	3.96	112.48	108.13
2	D	501	NAD	O4D-C1D-N1N	4.86	113.48	108.13
2	A	501	NAD	O4D-C1D-N1N	5.73	114.43	108.13

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

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

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	499/520 (95%)	-0.32	9 (1%)	71	71	10, 22, 41, 77	0
1	B	499/520 (95%)	-0.47	5 (1%)	84	84	9, 17, 34, 88	0
1	C	502/520 (96%)	-0.54	4 (0%)	87	87	9, 14, 28, 60	0
1	D	497/520 (95%)	-0.53	3 (0%)	90	90	9, 16, 32, 57	0
1	E	500/520 (96%)	-0.54	2 (0%)	93	92	8, 14, 28, 60	0
1	F	497/520 (95%)	-0.59	3 (0%)	90	90	8, 14, 26, 67	0
1	G	502/520 (96%)	-0.46	4 (0%)	87	87	10, 17, 31, 49	0
1	H	499/520 (95%)	-0.45	6 (1%)	81	81	9, 16, 30, 71	0
All	All	3995/4160 (96%)	-0.49	36 (0%)	85	85	8, 16, 33, 88	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-4	PHE	5.8
1	A	-1	ASN	5.3
1	C	-6	LEU	5.1
1	C	-5	TYR	5.0
1	B	-2	SER	4.6
1	H	-2	SER	4.5
1	B	-1	ASN	4.0
1	A	-2	SER	3.8
1	H	3	LEU	3.6
1	G	362	ASP	3.6
1	D	364	ASP	3.6
1	B	496	LYS	3.4
1	D	362	ASP	3.4
1	H	-1	ASN	3.3
1	G	364	ASP	3.2
1	F	362	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	495	SER	3.0
1	H	0	ALA	2.9
1	A	2	GLU	2.8
1	A	3	LEU	2.8
1	F	-1	ASN	2.7
1	B	362	ASP	2.7
1	A	365	ASP	2.5
1	G	-5	TYR	2.5
1	D	214	SER	2.5
1	A	5	LYS	2.3
1	C	362	ASP	2.3
1	F	364[A]	ASP	2.3
1	E	-1	ASN	2.2
1	A	0	ALA	2.1
1	A	311	ASP	2.1
1	G	307	GLN	2.1
1	A	6	HIS	2.0
1	H	2	GLU	2.0
1	H	362	ASP	2.0
1	C	364	ASP	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
1	CME	C	289[A]	10/11	0.95	0.11	-	14,16,31,32	10
1	CME	F	289[B]	10/11	0.97	0.09	-	13,15,24,26	10
1	CME	C	289[B]	10/11	0.95	0.11	-	13,15,24,25	10
1	CME	H	289[B]	10/11	0.94	0.12	-	20,24,31,31	10
1	CME	H	289[A]	10/11	0.94	0.12	-	20,23,40,41	10
1	CME	A	289	10/11	0.94	0.10	-	24,29,42,49	0
1	CME	D	289	10/11	0.94	0.10	-	17,24,43,59	0
1	CME	E	289[B]	10/11	0.97	0.12	-	15,19,31,31	10
1	CME	G	289[A]	10/11	0.94	0.14	-	20,22,34,35	10
1	CME	B	289[A]	10/11	0.97	0.08	-	15,18,30,32	10
1	CME	G	289[B]	10/11	0.94	0.14	-	20,24,35,35	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	F	289[A]	10/11	0.97	0.09	-	14,18,30,34	10
1	CME	E	289[A]	10/11	0.97	0.12	-	15,19,34,35	10
1	CME	B	289[B]	10/11	0.97	0.08	-	15,18,25,26	10

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(Å^2)	Q<0.9
3	NA	F	502	1/1	0.98	0.23	8.02	26,26,26,26	0
2	NAD	G	501	44/44	0.96	0.14	3.30	19,24,28,30	0
2	NAD	H	501	44/44	0.95	0.16	2.49	18,23,28,31	0
2	NAD	D	501	44/44	0.96	0.13	1.32	17,22,28,28	0
2	NAD	A	501	44/44	0.94	0.13	0.97	20,27,35,44	0
3	NA	H	502	1/1	0.99	0.08	0.69	14,14,14,14	0
3	NA	G	503	1/1	0.96	0.10	0.38	19,19,19,19	0
2	NAD	E	501	44/44	0.98	0.07	0.17	12,15,18,19	0
2	NAD	C	501	44/44	0.98	0.07	-0.06	12,14,18,18	0
2	NAD	F	501	44/44	0.99	0.07	-0.13	11,14,16,18	0
2	NAD	B	501	44/44	0.98	0.07	-0.39	13,17,19,22	0
3	NA	C	503	1/1	0.97	0.07	-0.99	16,16,16,16	0
3	NA	A	503	1/1	0.98	0.06	-1.25	19,19,19,19	0
3	NA	F	503	1/1	0.98	0.04	-2.13	14,14,14,14	0
3	NA	F	504	1/1	1.00	0.03	-2.16	8,8,8,8	0
3	NA	D	503	1/1	0.97	0.05	-2.19	18,18,18,18	0
3	NA	H	503	1/1	0.98	0.05	-2.24	16,16,16,16	0
3	NA	G	502	1/1	0.99	0.04	-2.43	15,15,15,15	0
3	NA	D	502	1/1	0.98	0.05	-2.59	12,12,12,12	0
3	NA	E	505	1/1	0.99	0.05	-2.68	16,16,16,16	0
3	NA	A	502	1/1	0.99	0.03	-3.14	17,17,17,17	0
3	NA	B	502	1/1	0.99	0.03	-3.21	13,13,13,13	0
3	NA	B	503	1/1	0.99	0.05	-3.40	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	C	502	1/1	0.99	0.04	-4.01	11,11,11,11	0
3	NA	E	504	1/1	1.00	0.02	-4.18	10,10,10,10	0
3	NA	E	503	1/1	0.79	0.19	-	31,31,31,31	0
3	NA	E	502	1/1	0.92	0.24	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.