

Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 - 05:27 PM EDT

PDB ID	:	4ZWL
Title	:	2.60 Angstrom resolution crystal structure of betaine aldehyde dehydrogenase
		(betB) H448F/Y450L double mutant from Staphylococcus aureus in complex
		with NAD+ and BME-free Cys289
Authors	:	Halavaty, A.S.; Minasov, G.; Chen, C.; Joo, J.C.; Yakunin, A.F.; Anderson,
		W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2015-05-19
Resolution	:	2.60 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 (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.35.1
:	1.1.7(2018)
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35.1
	: : : : : : : : : : : : : : : : : : : :



1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar resolution} \ (\# Entries, resolution range(Å))$		
R_{free}	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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	А	517	87%	9%	••
1	В	517	% 	7%	•
1	С	517	86%	10%	•
1	D	517	88%	8%	•
1	Е	517	90%	6%	•



Mol	Chain	Length	Quality of chain		
1	F	517	87%	8%	•••
1	G	517	87%	9%	•
1	Н	517	.% 88 %	8%	•



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32907 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	400	Total	С	Ν	0	S	0	10	0
1	A	499	3954	2492	667	780	15	0	10	0
1	р	400	Total	С	Ν	0	S	0	6	0
1	D	499	3916	2469	665	768	14	0	0	0
1	С	400	Total	С	Ν	0	S	0	7	0
1	U	499	3927	2475	665	773	14	0	1	0
1	а	408	Total	С	Ν	0	S	0	6	0
1	D	490	3912	2464	665	769	14	0	0	0
1	F	406	Total	С	Ν	0	S	0	10	0
1	Ľ	490	3929	2474	667	774	14	0	10	0
1	Б	406	Total	С	Ν	Ο	S	0	5	0
1	Г	490	3885	2449	658	764	14	0	5	0
1	С	406	Total	С	Ν	Ο	S	0	1	0
1	G	490	3876	2444	656	762	14	0	4	0
1	ц	406	Total	С	Ν	Ο	S	0	1	0
1	11	490	3877	2445	657	761	14	0	4	

• Molecule 1 is a protein called Betaine-aldehyde dehydrogenase.

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-20	MET	-	expression tag	UNP Q5HCU0
А	-19	GLY	-	expression tag	UNP Q5HCU0
А	-18	SER	-	expression tag	UNP Q5HCU0
А	-17	SER	-	expression tag	UNP Q5HCU0
A	-16	HIS	-	expression tag	UNP Q5HCU0
А	-15	HIS	-	expression tag	UNP Q5HCU0
A	-14	HIS	-	expression tag	UNP Q5HCU0
A	-13	HIS	-	expression tag	UNP Q5HCU0
А	-12	HIS	-	expression tag	UNP Q5HCU0
A	-11	HIS	-	expression tag	UNP Q5HCU0
A	-10	SER	-	expression tag	UNP Q5HCU0
A	-9	SER	-	expression tag	UNP Q5HCU0
А	-8	GLY	-	expression tag	UNP Q5HCU0



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Chain	Residue	Modelled	Actual	Comment	Reference
А	-7	ARG	-	expression tag	UNP Q5HCU0
А	-6	GLU	_	expression tag	UNP Q5HCU0
А	-5	ASN	_	expression tag	UNP Q5HCU0
А	-4	LEU	-	expression tag	UNP Q5HCU0
А	-3	TYR	_	expression tag	UNP Q5HCU0
А	-2	PHE	-	expression tag	UNP Q5HCU0
А	-1	GLN	_	expression tag	UNP Q5HCU0
А	0	GLY	_	expression tag	UNP Q5HCU0
А	448	PHE	HIS	engineered mutation	UNP Q5HCU0
А	450	LEU	TYR	engineered mutation	UNP Q5HCU0
В	-20	MET	_	expression tag	UNP Q5HCU0
В	-19	GLY	_	expression tag	UNP Q5HCU0
В	-18	SER	_	expression tag	UNP Q5HCU0
В	-17	SER	_	expression tag	UNP Q5HCU0
В	-16	HIS	_	expression tag	UNP Q5HCU0
В	-15	HIS	-	expression tag	UNP Q5HCU0
В	-14	HIS	_	expression tag	UNP Q5HCU0
В	-13	HIS	_	expression tag	UNP Q5HCU0
В	-12	HIS	_	expression tag	UNP Q5HCU0
В	-11	HIS	_	expression tag	UNP Q5HCU0
В	-10	SER	-	expression tag	UNP Q5HCU0
В	-9	SER	-	expression tag	UNP Q5HCU0
В	-8	GLY	_	expression tag	UNP Q5HCU0
В	-7	ARG	-	expression tag	UNP Q5HCU0
В	-6	GLU	-	expression tag	UNP Q5HCU0
В	-5	ASN	-	expression tag	UNP Q5HCU0
В	-4	LEU	-	expression tag	UNP Q5HCU0
В	-3	TYR	-	expression tag	UNP Q5HCU0
В	-2	PHE	-	expression tag	UNP Q5HCU0
В	-1	GLN	-	expression tag	UNP Q5HCU0
В	0	GLY	-	expression tag	UNP Q5HCU0
В	448	PHE	HIS	engineered mutation	UNP Q5HCU0
В	450	LEU	TYR	engineered mutation	UNP Q5HCU0
С	-20	MET	-	expression tag	UNP Q5HCU0
С	-19	GLY	-	expression tag	UNP Q5HCU0
С	-18	SER	-	expression tag	UNP Q5HCU0
С	-17	SER	-	expression tag	UNP Q5HCU0
С	-16	HIS	-	expression tag	UNP Q5HCU0
C	-15	HIS	-	expression tag	UNP Q5HCU0
С	-14	HIS	-	expression tag	UNP Q5HCU0
C	-13	HIS	-	expression tag	UNP Q5HCU0
С	-12	HIS	-	expression tag	UNP Q5HCU0

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Chain	Residue	Modelled	Actual	Comment	Reference
С	-11	HIS	-	expression tag	UNP Q5HCU0
С	-10	SER	-	expression tag	UNP Q5HCU0
С	-9	SER	-	expression tag	UNP Q5HCU0
С	-8	GLY	_	expression tag	UNP Q5HCU0
С	-7	ARG	_	expression tag	UNP Q5HCU0
С	-6	GLU	-	expression tag	UNP Q5HCU0
С	-5	ASN	-	expression tag	UNP Q5HCU0
С	-4	LEU	-	expression tag	UNP Q5HCU0
С	-3	TYR	-	expression tag	UNP Q5HCU0
С	-2	PHE	-	expression tag	UNP Q5HCU0
С	-1	GLN	-	expression tag	UNP Q5HCU0
С	0	GLY	-	expression tag	UNP Q5HCU0
С	448	PHE	HIS	engineered mutation	UNP Q5HCU0
С	450	LEU	TYR	engineered mutation	UNP Q5HCU0
D	-20	MET	-	expression tag	UNP Q5HCU0
D	-19	GLY	-	expression tag	UNP Q5HCU0
D	-18	SER	-	expression tag	UNP Q5HCU0
D	-17	SER	-	expression tag	UNP Q5HCU0
D	-16	HIS	-	expression tag	UNP Q5HCU0
D	-15	HIS	-	expression tag	UNP Q5HCU0
D	-14	HIS	-	expression tag	UNP Q5HCU0
D	-13	HIS	-	expression tag	UNP Q5HCU0
D	-12	HIS	-	expression tag	UNP Q5HCU0
D	-11	HIS	-	expression tag	UNP Q5HCU0
D	-10	SER	-	expression tag	UNP Q5HCU0
D	-9	SER	-	expression tag	UNP Q5HCU0
D	-8	GLY	-	expression tag	UNP Q5HCU0
D	-7	ARG	-	expression tag	UNP Q5HCU0
D	-6	GLU	-	expression tag	UNP Q5HCU0
D	-5	ASN	-	expression tag	UNP Q5HCU0
D	-4	LEU	-	expression tag	UNP Q5HCU0
D	-3	TYR	-	expression tag	UNP Q5HCU0
D	-2	PHE	-	expression tag	UNP Q5HCU0
D	-1	GLN	-	expression tag	UNP Q5HCU0
D	0	GLY	-	expression tag	UNP Q5HCU0
D	448	PHE	HIS	engineered mutation	UNP Q5HCU0
D	450	LEU	TYR	engineered mutation	UNP Q5HCU0
Е	-20	MET	-	expression tag	UNP Q5HCU0
Е	-19	GLY	-	expression tag	UNP Q5HCU0
Е	-18	SER	-	expression tag	UNP Q5HCU0
Е	-17	SER	-	expression tag	UNP Q5HCU0
Е	-16	HIS	-	expression tag	UNP Q5HCU0



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Reference
UNP Q5HCU0
UNP Q5HCU0
UNP Q5HCU0
UNP Q5HCU0

Chain	Residue	Modelled	Actual	Comment	Reference
Е	-15	HIS	-	expression tag	UNP Q5HCU0
Е	-14	HIS	-	expression tag	UNP Q5HCU0
Е	-13	HIS	-	expression tag	UNP Q5HCU0
Е	-12	HIS	-	expression tag	UNP Q5HCU0
Е	-11	HIS	-	expression tag	UNP Q5HCU0
Е	-10	SER	-	expression tag	UNP Q5HCU0
Е	-9	SER	-	expression tag	UNP Q5HCU0
Е	-8	GLY	-	expression tag	UNP Q5HCU0
Е	-7	ARG	-	expression tag	UNP Q5HCU0
Е	-6	GLU	-	expression tag	UNP Q5HCU0
Е	-5	ASN	-	expression tag	UNP Q5HCU0
Е	-4	LEU	-	expression tag	UNP Q5HCU0
Е	-3	TYR	-	expression tag	UNP Q5HCU0
Е	-2	PHE	-	expression tag	UNP Q5HCU0
Е	-1	GLN	-	expression tag	UNP Q5HCU0
Е	0	GLY	-	expression tag	UNP Q5HCU0
Е	448	PHE	HIS	engineered mutation	UNP Q5HCU0
Е	450	LEU	TYR	engineered mutation	UNP Q5HCU0
F	-20	MET	-	expression tag	UNP Q5HCU0
F	-19	GLY	-	expression tag	UNP Q5HCU0
F	-18	SER	-	expression tag	UNP Q5HCU0
F	-17	SER	-	expression tag	UNP Q5HCU0
F	-16	HIS	-	expression tag	UNP Q5HCU0
F	-15	HIS	-	expression tag	UNP Q5HCU0
F	-14	HIS	-	expression tag	UNP Q5HCU0
F	-13	HIS	-	expression tag	UNP Q5HCU0
F	-12	HIS	-	expression tag	UNP Q5HCU0
F	-11	HIS	-	expression tag	UNP Q5HCU0
F	-10	SER	-	expression tag	UNP Q5HCU0
F	-9	SER	-	expression tag	UNP Q5HCU0
F	-8	GLY	-	expression tag	UNP Q5HCU0
F	-7	ARG	-	expression tag	UNP Q5HCU0
F	-6	GLU	-	expression tag	UNP Q5HCU0
F	-5	ASN	-	expression tag	UNP Q5HCU0
F	-4	LEU	-	expression tag	UNP Q5HCU0
F	-3	TYR	-	expression tag	UNP Q5HCU0
F	-2	PHE	-	expression tag	UNP Q5HCU0
F	-1	GLN	-	expression tag	UNP Q5HCU0
F	0	GLY	-	expression tag	UNP Q5HCU0
F	448	PHE	HIS	engineered mutation	UNP Q5HCU0
F	450	LEU	TYR	engineered mutation	UNP Q5HCU0
G	-20	MET	-	expression tag	UNP Q5HCU0



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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	GLY	-	expression tag	UNP Q5HCU0
G	-18	SER	-	expression tag	UNP Q5HCU0
G	-17	SER	-	expression tag	UNP Q5HCU0
G	-16	HIS	-	expression tag	UNP Q5HCU0
G	-15	HIS	-	expression tag	UNP Q5HCU0
G	-14	HIS	-	expression tag	UNP Q5HCU0
G	-13	HIS	-	expression tag	UNP Q5HCU0
G	-12	HIS	-	expression tag	UNP Q5HCU0
G	-11	HIS	-	expression tag	UNP Q5HCU0
G	-10	SER	-	expression tag	UNP Q5HCU0
G	-9	SER	-	expression tag	UNP Q5HCU0
G	-8	GLY	-	expression tag	UNP Q5HCU0
G	-7	ARG	-	expression tag	UNP Q5HCU0
G	-6	GLU	-	expression tag	UNP Q5HCU0
G	-5	ASN	-	expression tag	UNP Q5HCU0
G	-4	LEU	-	expression tag	UNP Q5HCU0
G	-3	TYR	-	expression tag	UNP Q5HCU0
G	-2	PHE	-	expression tag	UNP Q5HCU0
G	-1	GLN	-	expression tag	UNP Q5HCU0
G	0	GLY	-	expression tag	UNP Q5HCU0
G	448	PHE	HIS	engineered mutation	UNP Q5HCU0
G	450	LEU	TYR	engineered mutation	UNP Q5HCU0
Н	-20	MET	-	expression tag	UNP Q5HCU0
Н	-19	GLY	-	expression tag	UNP Q5HCU0
Н	-18	SER	-	expression tag	UNP Q5HCU0
Н	-17	SER	-	expression tag	UNP Q5HCU0
Н	-16	HIS	-	expression tag	UNP Q5HCU0
Н	-15	HIS	-	expression tag	UNP Q5HCU0
Н	-14	HIS	-	expression tag	UNP Q5HCU0
H	-13	HIS	-	expression tag	UNP Q5HCU0
Н	-12	HIS	-	expression tag	UNP Q5HCU0
H	-11	HIS	-	expression tag	UNP Q5HCU0
Н	-10	SER	-	expression tag	UNP Q5HCU0
Н	-9	SER	-	expression tag	UNP Q5HCU0
H	-8	GLY	-	expression tag	UNP Q5HCU0
H	-7	ARG	-	expression tag	UNP Q5HCU0
Н	-6	GLU	-	expression tag	UNP Q5HCU0
Н	-5	ASN	-	expression tag	UNP Q5HCU0
H	-4	LEU	-	expression tag	UNP Q5HCU0
Н	-3	TYR	-	expression tag	UNP Q5HCU0
Н	-2	PHE	-	expression tag	UNP Q5HCU0
Н	-1	GLN	-	expression tag	UNP Q5HCU0

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Chain	Residue	Modelled	Actual	Comment	Reference			
Н	0	GLY	-	expression tag	UNP Q5HCU0			
Н	448	PHE	HIS	engineered mutation	UNP Q5HCU0			
Н	450	LEU	TYR	engineered mutation	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		Ate	oms			ZeroOcc	AltConf
0	Δ	1	Total	С	Ν	0	Р	0	0
	A	L	44	21	7	14	2	0	0
0	Р	1	Total	С	Ν	Ο	Р	0	0
	D	L	44	21	7	14	2	0	0
0	C	1	Total	С	Ν	0	Р	0	0
	U	L	44	21	7	14	2	0	0
0	Л	1	Total	С	Ν	Ο	Р	0	0
	D	L	44	21	7	14	2		
0	F	1	Total	С	Ν	0	Р	0	0
	Ľ	L	44	21	7	14	2	0	
9	F	1	Total	С	Ν	Ο	Р	0	0
	T,	T	44	21	7	14	2	0	0
9	G	1	Total	С	Ν	Ο	Р	0	0
2 G	1	44	21	7	14	2	U	U	
9	н	1	Total	С	Ν	Ο	Р	0	0
	11	L	44	21	7	14	2	U	





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	5	ZeroOcc	AltConf
3	G	1	Total O 5 4	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	177	Total O 180 180	0	5
4	В	182	Total O 183 183	0	2
4	С	166	Total O 168 168	0	3
4	D	174	Total O 176 176	0	3
4	Е	125	Total O 125 125	0	2
4	F	151	Total O 151 151	0	2
4	G	122	Total O 123 123	0	1
4	Н	98	Total O 98 98	0	1



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

• Molecule 1: Betaine-aldehyde dehydrogenase





• Molecule 1: Betaine-aldehyde dehydrogenase

Chain E:	90%		6% •
MET GLY SER SER HIS HIS HIS HIS SER ASN GLY CLY CLY CLY CLY CLY CLY CLY	R77 195 K100 Y158	11 01 11 02 12 05 12 52 12 52 1	1301 K317 V346 E350 V356 D362
R363 D364 D364 D365 D365 D365 D365 C410 C440 C440 C440 C440 C440 C440 C440			
• Molecule 1: Betaine-aldehyde d	lehydrogenas	e	
Chain F:	87%		8% • •
MET GLY GLY SER HIS HIS HIS SER ARS CLY CLY CLY CLY CLY CLY CLY	129 N30 K45 S105 M109	E129 E139 V150 V150 C158 C158 C158 T189 V162	C217 C217 D218 C219 C219 C219 C219 C228 N248 N248 N260
D266 D266 2291 1301 1301 1318 1334 1334 1334 1334 1334 1334 133	E399 6417 6431 8432 8433	1430 1447 1448 1449 1449 1449 1448 1488 1488 1488	
• Molecule 1: Betaine-aldehyde d	lehydrogenas	e	
Chain G:	87%		9% •
MET SER SER HIS HIS HIS HIS HIS SER HIS SER ASU ALY CLY CLY CLY CLY	K5 K45 K57 E67 R72	A80 195 196 197 197 116 116 1154 1154 1154	1100 1162 1173 1188 1188 1189 1189
C213 V219 V249 V249 C266 C286 C286 C286 C289 C286 C289 C286 C289 C286 C289 C286 C289 C286 C289 C286 C289 C286 C286 C286 C286 C286 C286 C286 C286	L370 G393 F401 A407 G417	G420 V433 V433 L437 E448 E448 P449 P449 L477	K496
• Molecule 1: Betaine-aldehyde d	lehydrogenas	e	





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	89.14Å 170.97Å 137.58Å	Depositor
a, b, c, α , β , γ	90.00° 102.77° 90.00°	Depositor
Bosolution(A)	29.95 - 2.60	Depositor
Resolution (A)	29.95 - 2.60	EDS
% Data completeness	99.9 (29.95-2.60)	Depositor
(in resolution range)	$100.0\ (29.95-2.60)$	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.46 (at 2.61 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
B B.	0.158 , 0.232	Depositor
n, n_{free}	0.163 , 0.232	DCC
R_{free} test set	6075 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 40.4	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32907	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SO4, 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		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.56	0/4025	0.86	1/5438~(0.0%)	
1	В	0.56	0/3991	0.84	0/5393	
1	С	0.53	0/3998	0.82	0/5403	
1	D	0.53	0/3982	0.80	1/5381~(0.0%)	
1	Е	0.52	0/4001	0.81	0/5406	
1	F	0.53	0/3955	0.82	0/5346	
1	G	0.50	0/3946	0.81	0/5334	
1	Н	0.49	0/3947	0.79	1/5335~(0.0%)	
All	All	0.53	0/31845	0.82	3/43036~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	259	LYS	N-CA-C	-5.53	96.06	111.00
1	А	354	ILE	N-CA-C	-5.49	96.17	111.00
1	Н	57	ARG	NE-CZ-NH1	5.17	122.88	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	${ m H(model)}$	H(added)	Clashes	Symm-Clashes
1	А	3954	0	3889	39	0
1	В	3916	0	3865	30	0
1	С	3927	0	3867	39	0
1	D	3912	0	3858	27	0
1	Е	3929	0	3871	27	0
1	F	3885	0	3834	35	0
1	G	3876	0	3828	29	0
1	Н	3877	0	3832	33	0
2	А	44	0	26	7	0
2	В	44	0	26	5	0
2	С	44	0	26	4	0
2	D	44	0	26	2	0
2	Е	44	0	26	5	0
2	F	44	0	26	5	0
2	G	44	0	26	2	0
2	Н	44	0	26	5	0
3	А	10	0	0	0	0
3	В	10	0	0	0	0
3	С	10	0	0	0	0
3	D	5	0	0	0	0
3	Е	10	0	0	0	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
4	А	180	0	0	4	0
4	В	183	0	0	5	0
4	С	168	0	0	4	0
4	D	176	0	0	3	0
4	Е	125	0	0	3	0
4	F	151	0	0	3	0
4	G	123	0	0	3	0
4	Н	98	0	0	6	0
All	All	32907	0	31052	246	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 4.

All (246) 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:431[A]:GLN:HG2	4:D:704[A]:HOH:O	1.26	1.25
1:E:289:CYS:SG	2:E:501:NAD:C4N	2.29	1.20
1:B:289:CYS:SG	2:B:501:NAD:C4N	2.38	1.11



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A + a 1	1 0 Adama 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:289:CYS:SG	2:A:501:NAD:C4N	2.42	1.07
1:F:289:CYS:SG	2:F:501:NAD:C4N	2.49	0.99
1:H:289:CYS:SG	2:H:501:NAD:C4N	2.52	0.97
1:C:289:CYS:SG	2:C:501:NAD:C4N	2.55	0.94
1:E:363:ARG:HD2	1:E:365:ASP:OD1	1.73	0.88
1:D:289:CYS:SG	2:D:501:NAD:C4N	2.64	0.85
1:F:431[A]:GLN:HG2	4:F:678[A]:HOH:O	1.76	0.83
1:E:317:LYS:HD2	4:E:722:HOH:O	1.82	0.78
1:E:289:CYS:SG	2:E:501:NAD:C3N	2.71	0.78
1:G:289:CYS:SG	2:G:501:NAD:C4N	2.73	0.77
1:A:353[A]:THR:HG23	4:A:622:HOH:O	1.84	0.77
1:A:289:CYS:SG	2:A:501:NAD:C3N	2.76	0.73
1:B:289:CYS:SG	2:B:501:NAD:H4N	2.27	0.73
1:C:289:CYS:SG	2:C:501:NAD:C3N	2.81	0.69
1:H:360:ARG:HB3	4:H:691:HOH:O	1.94	0.67
1:E:289:CYS:SG	2:E:501:NAD:H4N	2.33	0.67
1:E:289:CYS:SG	2:E:501:NAD:C5N	2.83	0.67
1:G:45:LYS:HB2	1:G:219:VAL:HG21	1.78	0.65
1:B:289:CYS:SG	2:B:501:NAD:C3N	2.86	0.64
1:A:150:VAL:HG12	1:A:228:LEU:HB3	1.81	0.63
1:D:450:LEU:O	1:D:450:LEU:HD12	1.99	0.63
1:E:266:ASP:HA	1:E:301:ILE:HD13	1.82	0.62
1:E:450:LEU:HD12	1:E:450:LEU:O	2.00	0.61
1:B:111:ASP:O	1:B:115:VAL:HG23	2.01	0.60
1:C:314:LYS:HE2	4:C:643:HOH:O	2.02	0.60
1:H:276:GLN:OE1	1:H:276:GLN:HA	2.02	0.59
1:C:150:VAL:HG12	1:C:228:LEU:HB3	1.83	0.59
1:F:483:LEU:HD22	1:G:449:PRO:HB2	1.84	0.59
1:A:363:ARG:NH2	1:A:365:ASP:OD1	2.35	0.59
1:A:307:GLN:HG3	4:A:761:HOH:O	2.03	0.58
1:D:449:PRO:HA	4:D:632:HOH:O	2.03	0.58
1:H:289:CYS:SG	2:H:501:NAD:C3N	2.91	0.58
1:C:314:LYS:CE	4:C:643:HOH:O	2.52	0.58
1:A:141:LYS:NZ	1:C:139:GLU:OE1	2.34	0.58
1:C:45:LYS:HB2	1:C:219:VAL:HG21	1.85	0.58
1:B:129:GLU:HA	1:D:129:GLU:HA	1.86	0.57
1:G:333:SER:HA	1:G:370:LEU:HD13	1.85	0.57
1:F:158:TYR:O	1:F:162:GLN:HG2	2.05	0.57
1:F:483:LEU:CD2	1:G:449:PRO:HB2	2.35	0.57
1:G:289:CYS:SG	2:G:501:NAD:C3N	2.92	0.57
1:H:22:ASN:OD1	1:H:24:ASN:HB3	2.05	0.57



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:150:VAL:HG12	1:H:228:LEU:HB3	1.86	0.57
1:G:420:GLY:HA3	1:G:439:LEU:HD13	1.87	0.56
1:D:447:PHE:O	1:D:448:PHE:HB2	2.06	0.56
1:A:129:GLU:HA	1:C:129:GLU:HA	1.87	0.56
1:C:368:ASP:OD1	4:C:601:HOH:O	2.16	0.56
1:E:1:MET:C	1:E:3:LEU:H	2.08	0.56
1:E:449:PRO:HB2	1:H:483:LEU:CD2	2.36	0.56
1:H:296:LEU:HD23	1:H:399:GLU:HB2	1.88	0.56
1:A:447:PHE:C	1:A:449:PRO:HD3	2.26	0.56
1:H:495:SER:O	4:H:601:HOH:O	2.18	0.55
1:H:168:ALA:HB3	1:H:169:PRO:HD3	1.89	0.55
1:B:260:ASN:HB2	1:B:291:ALA:O	2.06	0.55
1:A:483:LEU:HD22	1:D:449:PRO:HB2	1.89	0.55
1:B:425:LYS:HD2	4:B:734:HOH:O	2.05	0.55
1:E:77[A]:ARG:NH2	4:E:602:HOH:O	2.39	0.55
1:C:447:PHE:O	1:C:448:PHE:HB2	2.07	0.54
1:F:289:CYS:SG	2:F:501:NAD:C3N	2.95	0.54
1:H:22:ASN:OD1	1:H:24:ASN:CB	2.55	0.54
1:C:447:PHE:C	1:C:449:PRO:HD3	2.28	0.54
1:D:148:GLY:HA3	1:D:227:ASP:OD2	2.07	0.54
1:F:139:GLU:OE1	1:H:141:LYS:NZ	2.41	0.53
1:B:92:ARG:HD3	4:B:721:HOH:O	2.08	0.53
1:E:447:PHE:O	1:E:448:PHE:HB2	2.08	0.53
1:A:313:VAL:HG13	1:A:374:PRO:HB2	1.91	0.53
1:D:344:MET:O	1:D:348:LYS:HG3	2.08	0.53
1:F:129:GLU:HA	1:H:129:GLU:HA	1.89	0.53
1:B:450:LEU:O	1:B:450:LEU:HD12	2.10	0.52
1:E:447:PHE:C	1:E:449:PRO:HD3	2.30	0.52
1:F:260:ASN:HB2	1:F:291:ALA:O	2.08	0.52
1:A:266:ASP:OD2	1:A:300:SER:OG	2.28	0.52
1:D:495:SER:HA	4:D:765:HOH:O	2.10	0.52
1:A:257:GLY:HA2	2:A:501:NAD:O2D	2.10	0.52
1:H:233:GLY:O	1:H:256:LEU:HA	2.10	0.52
1:D:289:CYS:SG	2:D:501:NAD:C3N	2.97	0.51
1:H:447:PHE:C	1:H:449:PRO:HD3	2.31	0.51
1:F:289:CYS:SG	2:F:501:NAD:H4N	2.48	0.51
1:F:334:THR:HG22	1:F:370:LEU:HD21	1.93	0.51
1:B:346:VAL:O	1:B:350:GLU:HG2	2.10	0.50
1:F:150:VAL:HG12	1:F:228:LEU:HB3	1.92	0.50
1:B:57[A]:ARG:CZ	1:B:57[A]:ARG:HB3	2.41	0.50
1:F:432:ARG:O	1:F:436:LYS:HG2	2.11	0.50



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Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:D:288:VAL:HG12	1:D:290:SER:H	1.77	0.50
1:A:335[B]:GLU:OE1	1:A:335[B]:GLU:N	2.33	0.50
1:A:447:PHE:O	1:A:448:PHE:HB2	2.12	0.50
1:B:474:GLU:HG2	4:B:700:HOH:O	2.11	0.50
1:D:362:ASP:O	1:D:363:ARG:C	2.50	0.50
1:B:14:ASP:OD1	1:B:57[A]:ARG:NH1	2.44	0.50
1:G:97:ASP:HB2	1:G:187:LEU:HD12	1.93	0.49
1:F:296:LEU:HD23	1:F:399:GLU:HB2	1.94	0.49
1:B:112:ILE:HD13	1:B:160:LEU:HG	1.95	0.49
1:E:252:ILE:O	1:E:252:ILE:HG13	2.11	0.49
1:G:346:VAL:O	1:G:350:GLU:HG2	2.13	0.49
1:A:154:THR:OG1	1:A:181:PRO:HA	2.13	0.49
1:F:45:LYS:HB2	1:F:219:VAL:HG21	1.95	0.49
1:C:434:ALA:CB	1:C:442:VAL:HG11	2.42	0.49
1:G:286:GLY:HA3	1:G:393:GLY:O	2.12	0.49
1:F:344:MET:O	1:F:348:LYS:HG3	2.12	0.48
1:G:447:PHE:O	1:G:448:PHE:HB2	2.14	0.48
1:A:297:VAL:O	1:A:400:GLY:HA2	2.14	0.48
1:C:155:PRO:HB3	2:C:501:NAD:H52N	1.95	0.48
1:E:289:CYS:HB3	2:E:501:NAD:C6N	2.43	0.48
1:C:266:ASP:HA	1:C:301:ILE:HD13	1.95	0.48
1:F:449:PRO:HB2	1:G:483:LEU:HD22	1.95	0.48
1:F:431[A]:GLN:CG	4:F:678[A]:HOH:O	2.50	0.48
1:B:289:CYS:SG	2:B:501:NAD:C5N	3.01	0.48
1:F:289:CYS:SG	2:F:501:NAD:C5N	3.02	0.48
1:C:471:GLU:HG3	4:C:743:HOH:O	2.14	0.47
1:G:189:THR:HA	1:G:192:VAL:HG12	1.96	0.47
1:H:186:PRO:O	1:H:190:ILE:HG13	2.14	0.47
1:C:61:SER:HB3	1:C:63:GLU:OE2	2.14	0.47
1:C:45:LYS:O	1:C:49[A]:GLU:HG3	2.14	0.47
1:F:25:THR:HG23	4:F:602:HOH:O	2.14	0.47
1:F:248:ASN:O	1:F:249:VAL:C	2.53	0.47
1:A:339[A]:LYS:HE2	1:A:343:TYR:HE2	1.79	0.47
1:H:77[B]:ARG:HG3	1:H:117:MET:SD	2.54	0.47
1:B:88:GLU:HB3	4:B:633:HOH:O	2.14	0.47
1:B:331:VAL:HG22	1:B:370:LEU:O	2.15	0.47
1:F:333:SER:HA	1:F:370:LEU:HD13	1.95	0.47
1:G:335:GLU:HG3	4:G:705:HOH:O	2.14	0.47
1:H:331:VAL:HG22	1:H:370:LEU:O	2.15	0.47
1:C:362:ASP:N	1:C:362:ASP:OD1	2.47	0.47
1:C:333:SER:HA	1:C:370:LEU:HD13	1.97	0.47



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Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:H:95:THR:HG23	1:H:100:LYS:O	2.14	0.47
1:C:154:THR:HB	1:C:155:PRO:HD2	1.96	0.47
1:A:288:VAL:HG12	1:A:290:SER:H	1.79	0.46
1:C:158:TYR:O	1:C:162:GLN:HG2	2.16	0.46
1:A:289:CYS:SG	2:A:501:NAD:H4N	2.46	0.46
1:F:318:LEU:CD2	1:F:328:MET:HB3	2.46	0.46
1:C:14:ASP:CG	1:C:57:ARG:HH22	2.19	0.46
1:F:266:ASP:HA	1:F:301:ILE:HD13	1.98	0.46
1:A:449:PRO:HB2	1:D:483:LEU:HD22	1.97	0.46
1:E:440:GLY:HA3	1:E:457:GLY:O	2.15	0.46
1:D:111:ASP:O	1:D:115:VAL:HG23	2.15	0.46
1:F:189:THR:O	1:F:192:VAL:HG12	2.15	0.46
1:C:189:THR:O	1:C:192:VAL:HG12	2.16	0.46
1:F:150:VAL:HG23	1:F:150:VAL:O	2.16	0.46
1:C:186:PRO:O	1:C:190:ILE:HG13	2.15	0.46
1:C:62:GLY:O	1:C:63:GLU:C	2.54	0.45
1:G:433:VAL:O	1:G:437:LEU:HG	2.17	0.45
1:H:289:CYS:SG	2:H:501:NAD:H4N	2.52	0.45
1:B:62:GLY:HA2	1:B:65:SER:OG	2.17	0.45
1:H:334:THR:HG22	1:H:370:LEU:HD21	1.99	0.45
1:A:261:PRO:HA	1:A:294:ARG:O	2.17	0.45
1:A:289:CYS:SG	2:A:501:NAD:C5N	3.01	0.45
1:A:401:PHE:CD1	1:A:407:ALA:HB2	2.52	0.45
1:B:45:LYS:HB2	1:B:219:VAL:HG21	1.98	0.45
1:D:45:LYS:HB2	1:D:219:VAL:HG21	1.99	0.45
1:G:401:PHE:CD1	1:G:407:ALA:HB2	2.52	0.45
1:A:45:LYS:HD3	4:A:758:HOH:O	2.15	0.45
1:E:260:ASN:HB2	1:E:291:ALA:O	2.17	0.45
1:B:450:LEU:HD12	1:B:450:LEU:C	2.37	0.45
1:C:318:LEU:CD2	1:C:328:MET:HB3	2.47	0.45
1:A:448:PHE:N	1:A:449:PRO:CD	2.80	0.44
1:C:361:PRO:HG2	1:C:371:PHE:HB2	1.99	0.44
1:E:346:VAL:O	1:E:350:GLU:HG2	2.17	0.44
1:H:260:ASN:HB2	1:H:291:ALA:O	2.18	0.44
1:A:256:LEU:O	2:A:501:NAD:H2N	2.18	0.44
1:D:79:ILE:O	1:D:83:ILE:HG12	2.18	0.44
1:F:467:GLU:O	1:F:468:LEU:HB2	2.18	0.44
1:D:32:TYR:O	1:D:369:GLY:HA3	2.18	0.44
1:H:22:ASN:HA	4:H:645:HOH:O	2.18	0.43
1:H:289:CYS:HB3	2:H:501:NAD:C6N	2.49	0.43
1:H:61:SER:HA	4:H:677:HOH:O	2.19	0.43



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A + a 1		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:260:ASN:HB2	1:C:291:ALA:O	2.19	0.43	
1:G:95:THR:HG23	1:G:100:LYS:O	2.18	0.43	
1:A:333:SER:HA	1:A:370:LEU:HD13	1.99	0.43	
1:C:155:PRO:CB	2:C:501:NAD:H52N	2.49	0.43	
1:F:29:ILE:HG22	1:F:30:ASN:N	2.34	0.43	
1:B:266:ASP:HA	1:B:301:ILE:HD13	1.99	0.43	
1:G:2:GLU:O	1:G:5:LYS:HG2	2.18	0.43	
1:C:470:LYS:O	1:C:474[A]:GLU:HG3	2.19	0.43	
1:G:249:VAL:HG12	1:G:249:VAL:O	2.18	0.43	
1:C:434:ALA:HB1	1:C:442:VAL:HG11	2.00	0.43	
1:E:158:TYR:HB3	1:E:161:LEU:HB3	2.00	0.43	
1:E:236[B]:GLU:HG2	4:E:720:HOH:O	2.18	0.43	
1:A:288:VAL:HB	1:A:291:ALA:HB2	2.00	0.42	
1:C:233:GLY:O	1:C:256:LEU:HA	2.19	0.42	
1:H:10:ARG:HB3	1:H:18:VAL:O	2.19	0.42	
1:C:297:VAL:O	1:C:400:GLY:HA2	2.20	0.42	
1:D:186:PRO:O	1:D:190:ILE:HG13	2.20	0.42	
1:G:333:SER:CA	1:G:370:LEU:HD13	2.48	0.42	
1:H:266:ASP:HA	1:H:301:ILE:HD13	2.01	0.42	
1:D:62:GLY:HA2	1:D:65:SER:OG	2.19	0.42	
1:G:154:THR:HB	1:G:155:PRO:HD2	2.02	0.42	
1:B:148:GLY:HA3	1:B:227:ASP:OD2	2.19	0.42	
1:D:457:GLY:HA3	1:D:466:ARG:HD3	2.02	0.42	
1:G:80:ALA:HB2	1:G:116:PHE:HB3	2.02	0.42	
1:A:158:TYR:O	1:A:162:GLN:HG2	2.20	0.42	
1:A:374:PRO:HA	1:A:394:PRO:HB2	2.00	0.42	
1:G:173:THR:HB	1:G:477:LEU:HD21	2.01	0.42	
1:A:200:GLY:HA2	4:A:720:HOH:O	2.20	0.42	
1:E:95:THR:HG23	1:E:100:LYS:O	2.19	0.42	
1:C:14:ASP:OD2	1:C:57:ARG:NH2	2.53	0.42	
1:G:213:GLY:N	4:G:610:HOH:O	2.52	0.42	
1:F:447:PHE:O	1:F:448:PHE:HB2	2.20	0.42	
1:A:128:GLY:HA3	1:A:142:ILE:O	2.19	0.41	
1:D:447:PHE:O	1:D:448:PHE:CB	2.68	0.41	
1:E:490:LEU:HD12	1:E:490:LEU:N	2.35	0.41	
1:F:447:PHE:C	1:F:449:PRO:HD3	2.41	0.41	
1:H:447:PHE:O	1:H:448:PHE:HB2	2.20	0.41	
1:C:77[A]:ARG:HG3	1:C:117:MET:SD	2.61	0.41	
1:H:457:GLY:HA3	1:H:466:ARG:HD3	2.01	0.41	
1:B:59:PHE:CE1	1:B:148:GLY:HA2	2.55	0.41	
1:G:57:ARG:NH1	4:G:611:HOH:O	2.53	0.41	



$4\mathrm{Z}$	WL	
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A 4 1		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:H:289:CYS:SG	2:H:501:NAD:C5N	3.06	0.41	
1:A:296:LEU:HD23	1:A:399:GLU:HB2	2.02	0.41	
1:B:318:LEU:CD2	1:B:328:MET:HB3	2.51	0.41	
1:B:449:PRO:HG2	1:C:483:LEU:CD2	2.50	0.41	
1:C:334:THR:HG23	1:C:370:LEU:HD21	2.02	0.41	
1:E:356:VAL:HG12	1:E:376:VAL:HB	2.02	0.41	
1:B:257:GLY:HA2	2:B:501:NAD:O2D	2.21	0.41	
1:F:217:GLY:HA3	2:F:501:NAD:C2A	2.50	0.41	
1:F:333:SER:CA	1:F:370:LEU:HD13	2.51	0.41	
1:A:417:GLY:HA2	1:A:439:LEU:HD23	2.02	0.41	
1:C:492:ASN:OD1	1:C:496:LYS:HE3	2.21	0.41	
1:D:168:ALA:HB3	1:D:169:PRO:CD	2.51	0.41	
1:A:289:CYS:HB3	2:A:501:NAD:C6N	2.51	0.41	
1:B:168:ALA:HB3	1:B:169:PRO:HD3	2.03	0.41	
1:B:447:PHE:O	1:B:448:PHE:HB2	2.20	0.41	
1:D:77[A]:ARG:HG2	1:D:117:MET:SD	2.60	0.41	
1:D:224:LYS:HE3	1:D:224:LYS:HB2	1.83	0.41	
1:D:233:GLY:O	1:D:256:LEU:HA	2.21	0.41	
1:E:363:ARG:NH2	1:E:365:ASP:OD2	2.54	0.41	
1:H:301:ILE:HA	4:H:684:HOH:O	2.20	0.41	
1:E:1:MET:C	1:E:3:LEU:N	2.74	0.41	
1:E:362:ASP:OD1	1:E:362:ASP:C	2.58	0.41	
1:F:150:VAL:HG22	1:F:176:SER:O	2.21	0.41	
1:F:417:GLY:HA2	1:F:439:LEU:HD23	2.01	0.41	
1:G:158:TYR:O	1:G:162:GLN:HG2	2.21	0.41	
1:A:271[A]:GLU:OE1	1:A:271[A]:GLU:HA	2.21	0.40	
1:A:450:LEU:HD12	1:A:450:LEU:O	2.21	0.40	
1:G:117:MET:SD	1:H:77[B]:ARG:NH1	2.94	0.40	
1:B:179:MET:CG	1:B:180:LYS:N	2.84	0.40	
1:G:266:ASP:HA	1:G:301:ILE:HD13	2.02	0.40	
1:A:356:VAL:HG12	1:A:376:VAL:HB	2.04	0.40	
1:B:57[A]:ARG:HG2	4:B:679:HOH:O	2.21	0.40	
1:E:431:GLN:HG2	4:H:663:HOH:O	2.21	0.40	
1:H:148:GLY:HA3	1:H:227:ASP:OD2	2.21	0.40	
1:F:105:SER:O	1:F:109:MET:HG2	2.22	0.40	
1:G:67:GLU:O	1:G:72:ARG:NH1	2.55	0.40	
1:C:224:LYS:HE3	1:C:224:LYS:HB2	1.92	0.40	
1:D:231:PHE:CD1	1:D:241:ILE:CD1	3.04	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	Perce	entiles
1	А	507/517~(98%)	490 (97%)	14 (3%)	3 (1%)	25	47
1	В	503/517~(97%)	488 (97%)	13 (3%)	2(0%)	34	57
1	С	504/517~(98%)	483 (96%)	18 (4%)	3(1%)	25	47
1	D	502/517~(97%)	487 (97%)	12 (2%)	3(1%)	25	47
1	Е	504/517~(98%)	488 (97%)	15 (3%)	1 (0%)	47	71
1	F	499/517~(96%)	485 (97%)	11 (2%)	3~(1%)	25	47
1	G	498/517~(96%)	475 (95%)	21 (4%)	2(0%)	34	57
1	Н	498/517~(96%)	475 (95%)	20 (4%)	3 (1%)	25	47
All	All	4015/4136 (97%)	3871 (96%)	124 (3%)	20 (0%)	29	52

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	448	PHE
1	В	448	PHE
1	С	363	ARG
1	С	448	PHE
1	D	448	PHE
1	Е	448	PHE
1	F	448	PHE
1	G	448	PHE
1	Н	448	PHE
1	Н	247	ASN
1	А	363	ARG
1	D	363	ARG
1	А	417	GLY
1	D	417	GLY
1	F	417	GLY
1	В	417	GLY
1	G	417	GLY



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Mol	Chain	Res	Type
1	С	159	PRO
1	Н	417	GLY
1	F	249	VAL

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	\mathbf{ntiles}
1	А	423/429~(99%)	423 (100%)	0	100	100
1	В	419/429~(98%)	419 (100%)	0	100	100
1	С	420/429~(98%)	420 (100%)	0	100	100
1	D	418/429~(97%)	417 (100%)	1 (0%)	93	98
1	Е	421/429~(98%)	419 (100%)	2(0%)	88	96
1	F	416/429~(97%)	415 (100%)	1 (0%)	93	98
1	G	415/429~(97%)	415 (100%)	0	100	100
1	Н	415/429~(97%)	415 (100%)	0	100	100
All	All	3347/3432~(98%)	3343 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	146	PRO
1	Е	364	ASP
1	Е	450	LEU
1	F	450	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	В	431	GLN
1	С	251	ASN
1	С	409	GLN



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Mol	Chain	\mathbf{Res}	Type
1	F	435	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec	T:nl.	Bo	ond leng	ths	В	ond ang	les
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	С	501	-	42,48,48	0.99	2 (4%)	50,73,73	1.35	7 (14%)
2	NAD	А	501	-	42,48,48	0.98	2 (4%)	50,73,73	1.42	6 (12%)
3	SO4	G	503	-	4,4,4	0.39	0	6,6,6	0.13	0
3	SO4	В	502	-	4,4,4	0.15	0	6,6,6	0.54	0
3	SO4	G	502	-	4,4,4	0.39	0	$6,\!6,\!6$	0.37	0
3	SO4	F	502	-	4,4,4	0.37	0	$6,\!6,\!6$	0.26	0
2	NAD	Е	501	-	42,48,48	1.00	1 (2%)	50,73,73	1.42	4 (8%)
2	NAD	D	501	-	42,48,48	1.05	1 (2%)	50,73,73	1.24	4 (8%)
2	NAD	В	501	-	42,48,48	0.96	2 (4%)	50,73,73	1.53	6 (12%)
3	SO4	Е	503	-	4,4,4	0.41	0	6,6,6	0.50	0
3	SO4	Е	502	-	4,4,4	0.41	0	6,6,6	0.25	0



Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	G	501	-	42,48,48	1.11	2 (4%)	50,73,73	1.42	7 (14%)
3	SO4	F	504	-	4,4,4	0.37	0	$6,\!6,\!6$	0.39	0
2	NAD	Н	501	-	42,48,48	1.06	1 (2%)	50,73,73	1.36	7 (14%)
2	NAD	F	501	-	42,48,48	1.06	1 (2%)	50,73,73	1.27	3 (6%)
3	SO4	В	503	-	4,4,4	0.45	0	$6,\!6,\!6$	0.37	0
3	SO4	С	503	-	4,4,4	0.43	0	6,6,6	0.36	0
3	SO4	D	502	-	4,4,4	0.35	0	$6,\!6,\!6$	0.19	0
3	SO4	А	503	-	4,4,4	0.41	0	$6,\!6,\!6$	0.23	0
3	SO4	F	503	-	4,4,4	0.42	0	$6,\!6,\!6$	0.71	0
3	SO4	С	502	-	4,4,4	0.42	0	6,6,6	0.36	0
3	SO4	G	504	-	4,4,4	0.43	0	6,6,6	0.26	0
3	SO4	А	502	-	4,4,4	0.40	0	6,6,6	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	Е	501	-	-	6/26/62/62	0/5/5/5
2	NAD	С	501	-	-	6/26/62/62	0/5/5/5
2	NAD	G	501	-	-	4/26/62/62	0/5/5/5
2	NAD	А	501	-	-	3/26/62/62	0/5/5/5
2	NAD	Н	501	-	-	3/26/62/62	0/5/5/5
2	NAD	D	501	-	-	4/26/62/62	0/5/5/5
2	NAD	F	501	-	-	2/26/62/62	0/5/5/5
2	NAD	В	501	-	-	1/26/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	D	501	NAD	O7N-C7N	5.09	1.33	1.24
2	G	501	NAD	O7N-C7N	4.94	1.33	1.24
2	Н	501	NAD	O7N-C7N	4.69	1.33	1.24
2	F	501	NAD	O7N-C7N	4.65	1.33	1.24
2	Е	501	NAD	O7N-C7N	4.53	1.32	1.24
2	С	501	NAD	O7N-C7N	3.89	1.31	1.24
2	А	501	NAD	O7N-C7N	3.76	1.31	1.24
2	В	501	NAD	O7N-C7N	3.71	1.31	1.24
2	А	501	NAD	C2A-N3A	2.25	1.35	1.32



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	501	NAD	C2B-C1B	-2.21	1.50	1.53
2	G	501	NAD	C2B-C1B	-2.10	1.50	1.53
2	С	501	NAD	C2D-C1D	-2.08	1.50	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	501	NAD	N3A-C2A-N1A	-5.99	119.31	128.68
2	Е	501	NAD	N3A-C2A-N1A	-5.24	120.49	128.68
2	D	501	NAD	N3A-C2A-N1A	-5.02	120.83	128.68
2	А	501	NAD	N3A-C2A-N1A	-4.74	121.27	128.68
2	G	501	NAD	N3A-C2A-N1A	-4.37	121.85	128.68
2	С	501	NAD	N3A-C2A-N1A	-4.30	121.95	128.68
2	F	501	NAD	N3A-C2A-N1A	-4.25	122.04	128.68
2	Н	501	NAD	N3A-C2A-N1A	-4.25	122.04	128.68
2	Н	501	NAD	PN-O3-PA	-3.86	119.59	132.83
2	В	501	NAD	C3N-C7N-N7N	3.68	122.17	117.75
2	D	501	NAD	C1B-N9A-C4A	-3.59	120.34	126.64
2	G	501	NAD	C4A-C5A-N7A	-3.54	105.70	109.40
2	G	501	NAD	C1B-N9A-C4A	-3.45	120.58	126.64
2	Е	501	NAD	C1B-N9A-C4A	-3.44	120.59	126.64
2	В	501	NAD	C1B-N9A-C4A	-3.39	120.69	126.64
2	Н	501	NAD	O4B-C1B-C2B	-3.14	102.33	106.93
2	С	501	NAD	C3N-C7N-N7N	3.13	121.51	117.75
2	С	501	NAD	C4A-C5A-N7A	-3.11	106.15	109.40
2	В	501	NAD	O7N-C7N-N7N	-3.02	118.28	122.58
2	Е	501	NAD	PN-O3-PA	-3.02	122.46	132.83
2	В	501	NAD	O4D-C1D-C2D	-3.01	102.53	106.93
2	G	501	NAD	C3N-C7N-N7N	3.00	121.35	117.75
2	G	501	NAD	PN-O3-PA	-2.96	122.66	132.83
2	Н	501	NAD	O7N-C7N-N7N	-2.81	118.59	122.58
2	А	501	NAD	PN-O3-PA	-2.78	123.28	132.83
2	Е	501	NAD	C4A-C5A-N7A	-2.74	106.54	109.40
2	А	501	NAD	C1B-N9A-C4A	-2.70	121.89	126.64
2	Н	501	NAD	C3N-C7N-N7N	2.64	120.92	117.75
2	F	501	NAD	O4D-C1D-C2D	-2.49	103.29	106.93
2	D	501	NAD	PN-O3-PA	-2.46	124.39	132.83
2	А	501	NAD	C5N-C4N-C3N	-2.43	117.47	120.34
2	D	501	NAD	O7N-C7N-N7N	-2.42	119.14	122.58
2	А	501	NAD	C4A-C5A-N7A	-2.39	106.91	109.40
2	С	501	NAD	PN-O3-PA	-2.38	124.65	132.83
2	С	501	NAD	O4D-C4D-C5D	-2.30	101.80	109.37



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	501	NAD	O4B-C1B-C2B	-2.29	103.59	106.93
2	Н	501	NAD	C4A-C5A-N7A	-2.28	107.02	109.40
2	А	501	NAD	O4D-C4D-C5D	-2.26	101.92	109.37
2	G	501	NAD	C5A-C6A-N6A	2.23	123.75	120.35
2	F	501	NAD	C4A-C5A-N7A	-2.23	107.08	109.40
2	Н	501	NAD	O4D-C1D-C2D	-2.20	103.71	106.93
2	С	501	NAD	C1B-N9A-C4A	-2.17	122.84	126.64
2	В	501	NAD	PN-O3-PA	-2.04	125.81	132.83
2	G	501	NAD	O7N-C7N-N7N	-2.03	119.69	122.58

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	501	NAD	O4D-C4D-C5D-O5D
2	С	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	O4D-C4D-C5D-O5D
2	Е	501	NAD	O4D-C1D-N1N-C6N
2	F	501	NAD	PN-O3-PA-O5B
2	А	501	NAD	O4D-C4D-C5D-O5D
2	А	501	NAD	C3D-C4D-C5D-O5D
2	Е	501	NAD	O4D-C4D-C5D-O5D
2	Е	501	NAD	C3D-C4D-C5D-O5D
2	G	501	NAD	O4D-C4D-C5D-O5D
2	G	501	NAD	C3D-C4D-C5D-O5D
2	Н	501	NAD	O4D-C4D-C5D-O5D
2	Н	501	NAD	C3D-C4D-C5D-O5D
2	С	501	NAD	C3D-C4D-C5D-O5D
2	D	501	NAD	C3D-C4D-C5D-O5D
2	В	501	NAD	C4D-C5D-O5D-PN
2	G	501	NAD	C4D-C5D-O5D-PN
2	F	501	NAD	C4D-C5D-O5D-PN
2	С	501	NAD	C5B-O5B-PA-O3
2	D	501	NAD	C5B-O5B-PA-O3
2	Е	501	NAD	C5B-O5B-PA-O3
2	G	501	NAD	C5B-O5B-PA-O3
2	А	501	NAD	C4D-C5D-O5D-PN
2	Н	501	NAD	C4D-C5D-O5D-PN
2	С	501	NAD	C4D-C5D-O5D-PN
2	D	501	NAD	C4D-C5D-O5D-PN
2	Е	501	NAD	C4D-C5D-O5D-PN
2	С	501	NAD	C5B-O5B-PA-O1A



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Mol	Chain	Res	Type	Atoms
2	Ε	501	NAD	C5B-O5B-PA-O1A

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	501	NAD	4	0
2	А	501	NAD	7	0
2	Е	501	NAD	5	0
2	D	501	NAD	2	0
2	В	501	NAD	5	0
2	G	501	NAD	2	0
2	Н	501	NAD	5	0
2	F	501	NAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

































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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	499/517~(96%)	-0.83	2 (0%) 92 91	20, 30, 47, 122	0
1	В	499/517~(96%)	-0.82	4 (0%) 86 84	20, 31, 48, 87	0
1	С	499/517~(96%)	-0.80	0 100 100	22, 34, 55, 80	0
1	D	498/517~(96%)	-0.75	0 100 100	22, 35, 54, 102	0
1	Е	496/517~(95%)	-0.67	2 (0%) 92 91	20, 35, 57, 98	0
1	F	496/517~(95%)	-0.75	1 (0%) 95 95	20, 34, 54, 93	0
1	G	496/517~(95%)	-0.60	2 (0%) 92 91	26, 41, 63, 104	0
1	Н	496/517~(95%)	-0.56	3 (0%) 89 88	24, 44, 70, 111	0
All	All	3979/4136~(96%)	-0.72	14 (0%) 92 91	20, 35, 60, 122	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	-1	GLN	3.8
1	В	496	LYS	3.2
1	Ε	163	ALA	2.9
1	В	-2	PHE	2.6
1	Н	368	ASP	2.4
1	Н	163	ALA	2.4
1	G	5	LYS	2.3
1	F	1	MET	2.2
1	В	-1	GLN	2.2
1	В	1	MET	2.2
1	А	0	GLY	2.2
1	Н	1	MET	2.2
1	Е	1	MET	2.2
1	G	368	ASP	2.1



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 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
3	SO4	С	502	5/5	0.78	0.38	75,89,99,124	0
3	SO4	F	504	5/5	0.80	0.45	70,72,75,86	5
3	SO4	F	502	5/5	0.83	0.28	58,93,97,107	0
3	SO4	А	502	5/5	0.85	0.37	61,62,78,80	5
3	SO4	Е	502	5/5	0.89	0.23	75,76,91,106	0
3	SO4	Е	503	5/5	0.90	0.27	60,67,78,85	0
3	SO4	G	503	5/5	0.91	0.28	62,65,71,73	5
3	SO4	В	503	5/5	0.92	0.20	46,69,76,83	0
3	SO4	С	503	5/5	0.94	0.18	49,58,67,80	0
3	SO4	G	502	5/5	0.95	0.19	42,49,64,66	5
2	NAD	D	501	44/44	0.96	0.12	26,36,41,45	0
3	SO4	F	503	5/5	0.96	0.15	37,42,52,53	0
3	SO4	D	502	5/5	0.96	0.24	46,47,57,60	5
2	NAD	G	501	44/44	0.96	0.12	23,37,48,60	0
2	NAD	Н	501	44/44	0.96	0.12	$29,\!41,\!51,\!57$	0
3	SO4	G	504	5/5	0.96	0.24	48,51,57,62	5
2	NAD	А	501	44/44	0.97	0.10	21,30,38,41	0
2	NAD	Е	501	44/44	0.97	0.11	22,38,45,49	0
3	SO4	А	503	5/5	0.97	0.11	36,43,48,51	0
2	NAD	F	501	44/44	0.97	0.09	18,30,35,38	0
2	NAD	С	501	44/44	0.97	0.10	25,33,44,50	0
2	NAD	В	501	44/44	0.98	0.09	17,29,35,40	0
3	SO4	В	502	5/5	0.98	0.14	39,42,48,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.













6.5 Other polymers (i)

There are no such residues in this entry.

