



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 05:29 AM GMT

PDB ID : 1I3K  
Title : MOLECULAR BASIS FOR SEVERE EPIMERASE-DEFICIENCY GALACTOSEMIA: X-RAY STRUCTURE OF THE HUMAN V94M-SUBSTITUTED UDP-GALACTOSE 4-EPIMERASE  
Authors : Thoden, J.B.; Wohlers, T.M.; Fridovich-Keil, J.L.; Holden, H.M.  
Deposited on : 2001-02-15  
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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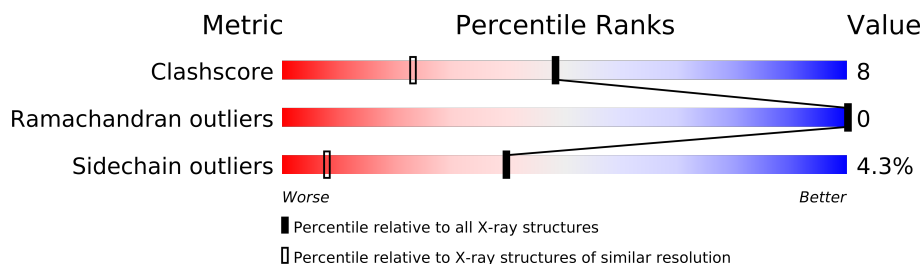
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6568 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UDP-GLUCOSE 4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	3	0
			2697	1706	467	508	16			
1	B	345	Total	C	N	O	S	0	12	0
			2716	1723	465	511	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	VAL	ENGINEERED	UNP Q14376
B	94	MET	VAL	ENGINEERED	UNP Q14376

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cl	0	0
			3	3		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

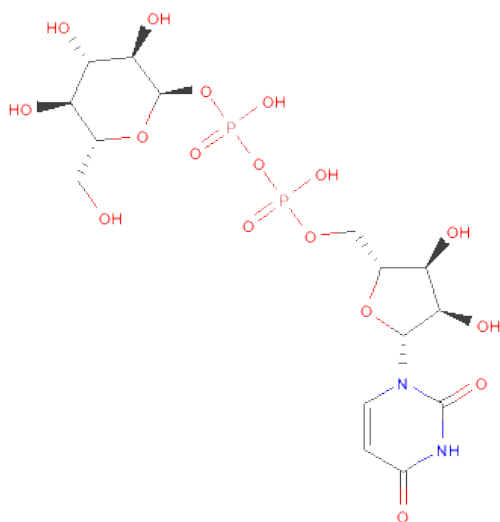
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 5 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula:  $C_{15}H_{24}N_2O_{17}P_2$ ).



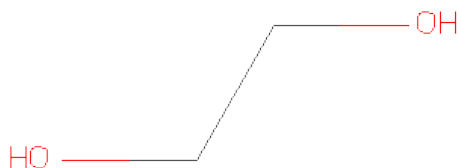
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			37	15	2	18	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	494	Total	O	0	0
			494	494		
7	B	483	Total	O	0	0
			483	483		

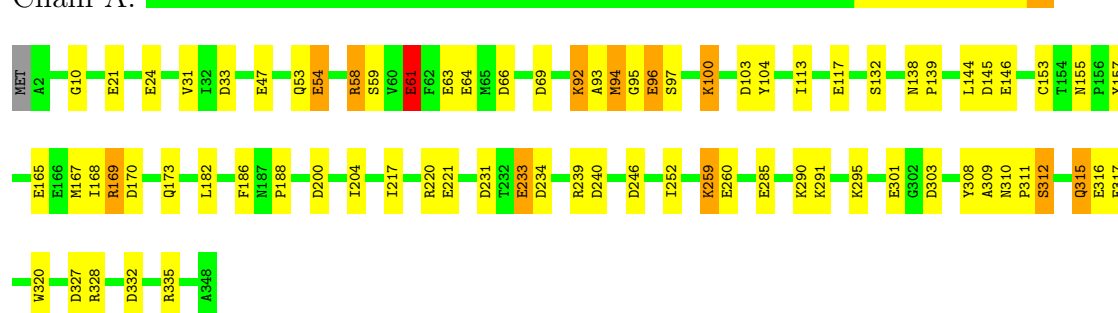
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain A:



#### • Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.10Å 89.90Å 96.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50	Depositor
% Data completeness (in resolution range)	99.1 (50.00-1.50)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , 0.198	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UPG, MG, EDO, NAD, CL

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	0.89	20/2766 (0.7%)	1.21	26/3740 (0.7%)
1	B	0.89	19/2825 (0.7%)	1.23	30/3821 (0.8%)
All	All	0.89	39/5591 (0.7%)	1.22	56/7561 (0.7%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63[A]	GLU	CD-OE2	6.67	1.32	1.25
1	A	63[B]	GLU	CD-OE2	6.67	1.32	1.25
1	B	317	GLU	CD-OE2	6.57	1.32	1.25
1	A	233	GLU	CD-OE2	6.57	1.32	1.25
1	B	63	GLU	CD-OE2	6.49	1.32	1.25
1	A	301	GLU	CD-OE2	6.46	1.32	1.25
1	A	47	GLU	CD-OE2	6.39	1.32	1.25
1	B	96	GLU	CD-OE2	6.35	1.32	1.25
1	A	146	GLU	CD-OE2	6.34	1.32	1.25
1	B	146	GLU	CD-OE2	6.24	1.32	1.25
1	A	260	GLU	CD-OE2	6.22	1.32	1.25
1	B	24	GLU	CD-OE2	6.11	1.32	1.25
1	A	317	GLU	CD-OE2	6.03	1.32	1.25
1	B	301	GLU	CD-OE2	6.01	1.32	1.25
1	A	316	GLU	CD-OE2	5.99	1.32	1.25
1	A	21	GLU	CD-OE2	5.94	1.32	1.25
1	B	3	GLU	CD-OE2	5.90	1.32	1.25
1	B	285	GLU	CD-OE2	5.78	1.32	1.25
1	B	54	GLU	CD-OE2	5.77	1.31	1.25
1	B	47	GLU	CD-OE2	5.72	1.31	1.25
1	B	165	GLU	CD-OE2	5.67	1.31	1.25
1	A	165	GLU	CD-OE2	5.67	1.31	1.25
1	A	117	GLU	CD-OE2	5.64	1.31	1.25
1	A	221	GLU	CD-OE2	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	GLU	CD-OE2	5.58	1.31	1.25
1	B	260	GLU	CD-OE2	5.52	1.31	1.25
1	B	21	GLU	CD-OE2	5.48	1.31	1.25
1	A	54	GLU	CD-OE2	5.45	1.31	1.25
1	B	233[A]	GLU	CD-OE2	5.42	1.31	1.25
1	B	233[B]	GLU	CD-OE2	5.42	1.31	1.25
1	A	61	GLU	CD-OE2	5.37	1.31	1.25
1	A	96	GLU	CD-OE2	5.37	1.31	1.25
1	A	285	GLU	CD-OE2	5.37	1.31	1.25
1	B	221	GLU	CD-OE2	5.33	1.31	1.25
1	A	24[A]	GLU	CD-OE2	5.31	1.31	1.25
1	A	24[B]	GLU	CD-OE2	5.31	1.31	1.25
1	B	61[A]	GLU	CD-OE2	5.27	1.31	1.25
1	B	61[B]	GLU	CD-OE2	5.27	1.31	1.25
1	B	316	GLU	CD-OE2	5.11	1.31	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	145	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	A	303	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	B	170	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	66	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	145	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	69	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	B	332	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	303	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	A	69	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	246	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	332	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	246	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	246	ASP	CB-CG-OD1	6.72	124.34	118.30
1	A	66	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	145	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	75	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	335	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	69	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	145	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	69	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	303	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	327	ASP	CB-CG-OD2	-6.12	112.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	50	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	200	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	335	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	332	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	B	170	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	66	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	200	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	234	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	239	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	327	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	92	LYS	N-CA-CB	5.68	120.82	110.60
1	A	170	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	231	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	246	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	303	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	327	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	268	ASN	CB-CA-C	-5.28	99.84	110.40
1	B	231[A]	ASP	CB-CG-OD1	5.25	123.02	118.30
1	B	231[B]	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	92	LYS	C-N-CA	-5.24	108.60	121.70
1	B	239	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	33	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	13	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	58	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	309	ALA	CB-CA-C	-5.13	102.40	110.10
1	B	50	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	231[A]	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	231[B]	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	200	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	132	SER	N-CA-CB	-5.05	102.92	110.50
1	B	300	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	234	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2697	0	2648	41	0
1	B	2716	0	2677	43	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
4	A	44	0	26	3	0
4	B	44	0	26	1	0
5	A	37	0	6	1	0
5	B	36	0	22	2	0
6	A	4	0	6	0	0
6	B	8	0	12	4	0
7	A	494	0	0	10	0
7	B	483	0	0	8	0
All	All	6568	0	5423	86	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:MET:HB3	1:A:96:GLU:HG3	1.44	0.97
1:B:58:ARG:HG3	1:B:58:ARG:HH11	1.38	0.89
1:B:94:MET:HB2	1:B:96:GLU:HG3	1.61	0.82
1:A:94:MET:HB3	1:A:96:GLU:CG	2.09	0.81
1:B:63:GLU:HG3	7:B:3032:HOH:O	1.83	0.78
1:B:83[B]:MET:HE1	1:B:259:LYS:HE2	1.66	0.77
1:B:42:GLY:HA2	7:B:1882:HOH:O	1.85	0.77
1:A:94:MET:HB2	7:A:2066:HOH:O	1.88	0.73
1:B:58:ARG:HG3	1:B:58:ARG:NH1	2.06	0.70
1:A:97:SER:HA	1:A:104:TYR:CE1	2.27	0.70
1:A:100:LYS:HE2	1:A:103:ASP:OD1	1.93	0.69
1:A:259:LYS:HD3	7:A:1620:HOH:O	1.94	0.67
1:B:100:LYS:HD3	1:B:103:ASP:HB2	1.77	0.66
1:A:155:ASN:OD1	1:A:157:TYR:HB3	1.96	0.65
1:A:61:GLU:HG2	7:A:1586:HOH:O	1.95	0.65
1:A:153:CYS:HB3	7:A:2072:HOH:O	1.97	0.64
1:A:312:SER:HA	1:A:315:GLN:CG	2.26	0.64
1:B:155:ASN:OD1	1:B:157:TYR:HB3	1.98	0.64
1:B:100:LYS:HD2	1:B:104:TYR:CE1	2.33	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:70:GLN:HG2	7:B:2011:HOH:O	1.98	0.63
1:A:290:LYS:NZ	7:A:3037:HOH:O	2.32	0.62
1:A:58:ARG:NH1	7:A:1843:HOH:O	2.31	0.61
1:B:78:LYS:HD2	6:B:972:EDO:O2	2.00	0.60
1:A:54:GLU:HG3	7:A:1850:HOH:O	2.01	0.60
1:B:310:ASN:C	1:B:310:ASN:HD22	2.07	0.58
1:B:94:MET:HB2	1:B:96:GLU:CG	2.32	0.58
1:A:217:ILE:HG13	1:A:217:ILE:O	2.03	0.57
1:A:188:PRO:HD2	4:A:400:NAD:O7N	2.05	0.57
1:B:310:ASN:HD22	1:B:312:SER:H	1.53	0.57
1:A:290:LYS:HE3	7:A:3009:HOH:O	2.04	0.56
1:B:310:ASN:ND2	1:B:312:SER:H	2.04	0.56
1:A:113:ILE:HG12	1:A:167:MET:HE1	1.88	0.55
1:B:100:LYS:HD2	1:B:104:TYR:HE1	1.71	0.55
1:B:155:ASN:H	1:B:155:ASN:HD22	1.56	0.53
1:B:74:GLN:HB3	6:B:972:EDO:H12	1.90	0.53
1:B:132:SER:OG	5:B:901:UPG:O4'	2.27	0.52
1:A:311:PRO:O	1:A:315:GLN:HG2	2.09	0.52
1:A:139:PRO:HB3	1:A:144:LEU:HD21	1.92	0.51
1:A:10:GLY:HA3	1:A:31:VAL:HG13	1.92	0.50
4:B:900:NAD:H4N	5:B:901:UPG:H4'	1.94	0.50
1:B:56:THR:O	1:B:58:ARG:NH1	2.44	0.50
1:B:97:SER:HA	1:B:104:TYR:CE1	2.46	0.50
1:A:93:ALA:C	1:A:95:GLY:H	2.15	0.49
1:B:70:GLN:HG3	7:B:1346:HOH:O	2.12	0.49
1:B:114:GLN:HB3	7:B:2011:HOH:O	2.13	0.48
1:B:53:GLN:HG3	1:B:58:ARG:O	2.13	0.48
1:B:240:ASP:HB2	1:B:308:TYR:HA	1.96	0.47
1:B:100:LYS:HE2	1:B:103:ASP:OD1	2.13	0.47
1:B:2:ALA:HB3	1:B:81[B]:SER:HB3	1.97	0.47
1:A:310:ASN:OD1	1:A:312:SER:OG	2.33	0.46
1:B:155:ASN:HD22	1:B:155:ASN:N	2.12	0.46
1:A:94:MET:HB3	1:A:96:GLU:OE2	2.15	0.46
1:A:186:PHE:O	5:A:401[A]:UPG:H6'1	2.15	0.46
1:A:240:ASP:HB2	1:A:308:TYR:HA	1.98	0.46
1:A:315:GLN:HA	1:A:320:TRP:O	2.16	0.45
1:B:2:ALA:N	1:B:82:PHE:O	2.50	0.45
1:A:167:MET:HB3	1:A:167:MET:HE3	1.78	0.45
1:B:186:PHE:CE2	1:B:309:ALA:HB2	2.52	0.45
1:A:173:GLN:OE1	1:A:173:GLN:HA	2.17	0.45
1:B:10:GLY:HA3	1:B:31:VAL:HG13	1.99	0.44
1:B:153:CYS:HB3	7:B:1318:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:ARG:HA	1:A:328:ARG:HD2	1.81	0.44
1:A:132:SER:HB2	4:A:400:NAD:H5N	1.99	0.44
1:B:74:GLN:CB	6:B:972:EDO:H12	2.49	0.43
1:B:83[B]:MET:CE	1:B:259:LYS:HE2	2.43	0.43
1:A:94:MET:HG3	1:A:94:MET:O	2.18	0.43
1:B:155:ASN:ND2	1:B:155:ASN:H	2.16	0.43
1:B:215:VAL:HG22	1:B:220:ARG:HB2	2.01	0.43
1:A:169:ARG:HD3	7:A:1507:HOH:O	2.20	0.42
1:A:312:SER:HA	1:A:315:GLN:HG2	2.00	0.42
1:B:75:ARG:HD2	7:B:1737:HOH:O	2.18	0.42
1:A:169:ARG:HD3	1:A:169:ARG:HH11	1.68	0.42
1:A:252:ILE:HD12	1:A:252:ILE:N	2.35	0.41
1:B:100:LYS:NZ	7:B:1959:HOH:O	2.47	0.41
1:B:74:GLN:HB3	6:B:972:EDO:C1	2.51	0.41
1:A:291:LYS:NZ	7:A:1374:HOH:O	2.53	0.41
1:A:94:MET:CB	1:A:96:GLU:HG3	2.32	0.41
1:A:53:GLN:HG3	1:A:58:ARG:O	2.20	0.40
1:A:315:GLN:HG2	1:A:315:GLN:H	1.69	0.40
1:B:35:PHE:CE2	1:B:40:ARG:HG3	2.55	0.40
1:B:4:LYS:NZ	1:B:28:LEU:HD13	2.37	0.40
1:A:204:ILE:HG12	1:A:220:ARG:NH1	2.36	0.40
1:B:272:GLY:HA2	1:B:309:ALA:O	2.21	0.40
1:A:168:ILE:HG21	1:A:182:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/348 (100%)	340 (98%)	8 (2%)	0	100	100
1	B	356/348 (102%)	349 (98%)	7 (2%)	0	100	100
All	All	704/696 (101%)	689 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	283/282 (100%)	271 (96%)	12 (4%)	40	8
1	B	292/282 (104%)	277 (95%)	15 (5%)	33	6
All	All	575/564 (102%)	548 (95%)	27 (5%)	40	6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	61	GLU
1	A	92	LYS
1	A	94	MET
1	A	100	LYS
1	A	138	ASN
1	A	169	ARG
1	A	233	GLU
1	A	259	LYS
1	A	295	LYS
1	A	312	SER
1	A	315	GLN
1	B	44	SER
1	B	58	ARG
1	B	81[A]	SER
1	B	81[B]	SER
1	B	100	LYS
1	B	153	CYS
1	B	155	ASN
1	B	159	LYS
1	B	217[A]	ILE
1	B	217[B]	ILE
1	B	233[A]	GLU
1	B	233[B]	GLU
1	B	301	GLU
1	B	304	VAL
1	B	310	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	206	ASN
1	A	224	ASN
1	A	337	GLN
1	A	339	GLN
1	B	36	HIS
1	B	70	GLN
1	B	114	GLN
1	B	138	ASN
1	B	206	ASN
1	B	224	ASN
1	B	310	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic and 2 are modelled with single atom - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAD	A	400	-	48,48,48	0.98	4 (8%)	73,73,73	1.45	7 (9%)
6	EDO	A	971	-	3,3,3	0.49	0	2,2,2	0.27	0
4	NAD	B	900	-	48,48,48	1.06	3 (6%)	73,73,73	1.37	7 (9%)
5	UPG	B	901	-	38,38,38	0.93	2 (5%)	54,58,58	0.98	4 (7%)
6	EDO	B	970	-	3,3,3	0.40	0	2,2,2	0.47	0
6	EDO	B	972	-	3,3,3	0.43	0	2,2,2	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	A	400	-	-	0/30/62/62	0/3/5/5
6	EDO	A	971	-	-	0/1/1/1	0/0/0/0
4	NAD	B	900	-	-	0/30/62/62	0/3/5/5
5	UPG	B	901	-	-	0/21/59/59	0/3/3/3
6	EDO	B	970	-	-	0/1/1/1	0/0/0/0
6	EDO	B	972	-	-	0/1/1/1	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	NAD	C4N-C3N	3.58	1.45	1.39
4	A	400	NAD	C2N-N1N	2.83	1.38	1.35
5	B	901	UPG	C6-C5	-2.52	1.31	1.36
4	B	900	NAD	C2N-N1N	2.33	1.38	1.35
4	A	400	NAD	C4N-C3N	2.28	1.43	1.39
4	B	900	NAD	PA-O2A	-2.18	1.45	1.55
5	B	901	UPG	C6-N1	2.14	1.39	1.35
4	A	400	NAD	C2A-N1A	2.05	1.38	1.33
4	A	400	NAD	PA-O2A	-2.04	1.45	1.55

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	NAD	C5N-C4N-C3N	-6.32	112.11	120.32
4	A	400	NAD	C5N-C6N-N1N	-4.68	112.55	120.43
4	B	900	NAD	C5N-C6N-N1N	-4.40	113.02	120.43
4	A	400	NAD	C6N-C5N-C4N	4.26	126.21	119.44
4	B	900	NAD	C5N-C4N-C3N	-4.13	114.95	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	NAD	C6N-C5N-C4N	3.78	125.45	119.44
4	A	400	NAD	O4D-C1D-N1N	3.34	111.36	107.95
4	B	900	NAD	C6N-N1N-C2N	3.29	125.75	122.04
4	A	400	NAD	C2N-C3N-C4N	2.92	121.62	118.31
4	B	900	NAD	C3N-C7N-N7N	2.88	121.04	117.77
5	B	901	UPG	O3B-C1'-C2'	2.82	113.55	108.38
4	B	900	NAD	C4A-C5A-N7A	2.63	111.78	109.52
5	B	901	UPG	C4'-C3'-C2'	-2.45	106.29	110.82
4	B	900	NAD	N6A-C6A-N1A	2.22	123.72	119.36
5	B	901	UPG	PB-O3B-C1'	-2.20	110.26	119.58
4	A	400	NAD	O4B-C1B-C2B	-2.17	103.44	106.77
5	B	901	UPG	O5'-C1'-O3B	2.13	114.14	111.36
4	A	400	NAD	O4B-C1B-N9A	-2.12	106.47	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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