



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:42 AM GMT

PDB ID : 3BTO  
Title : HORSE LIVER ALCOHOL DEHYDROGENASE COMPLEXED TO NADH  
AND (1S,3S)3-BUTYLTHIOLANE 1-OXIDE  
Authors : Ramaswamy, S.; Plapp, B.V.  
Deposited on : 1996-11-08  
Resolution : 1.66 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (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

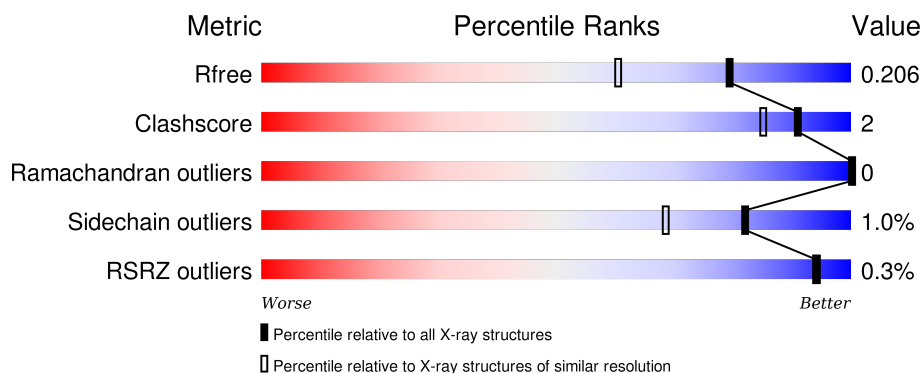
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	<div> <div>86%</div> <div>14%</div> </div>
1	B	374	<div> <div>86%</div> <div>13%</div> <div>•</div> </div>
1	C	374	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
1	D	374	<div> <div>%</div> <div>91%</div> <div>9%</div> <div>•</div> </div>

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
4	SSB	C	378	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12979 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 LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	B	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	C	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	D	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

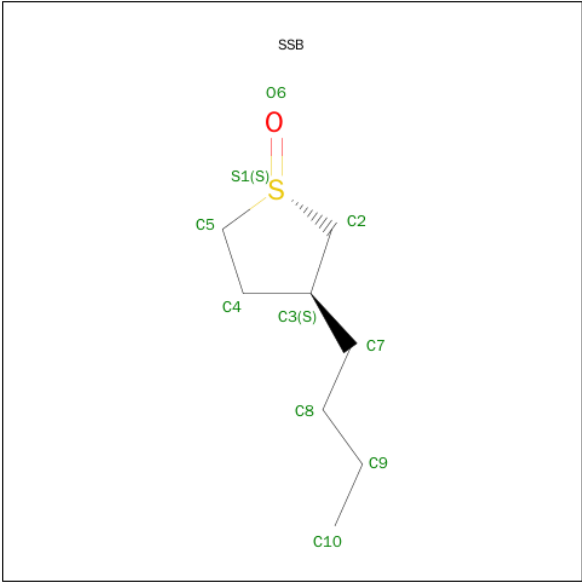
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 3-BUTYLTHIOLANE 1-OXIDE (three-letter code: SSB) (formula: C<sub>8</sub>H<sub>16</sub>OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 10 8 1 1	0	0
4	B	1	Total C O S 10 8 1 1	0	0
4	C	1	Total C O S 10 8 1 1	0	0
4	D	1	Total C O S 10 8 1 1	0	0

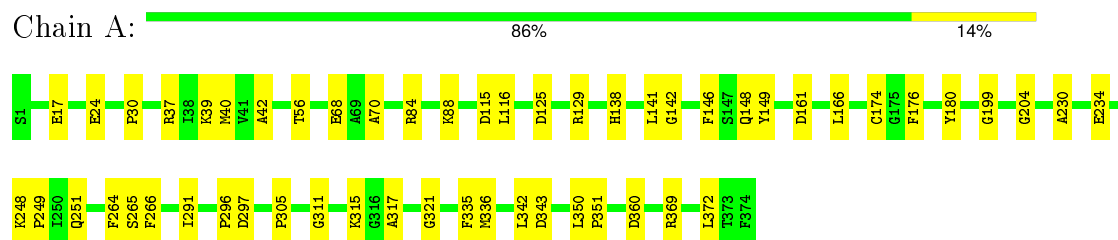
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	376	Total O 376 376	0	0
5	B	437	Total O 437 437	0	0
5	C	406	Total O 406 406	0	0
5	D	396	Total O 396 396	0	0

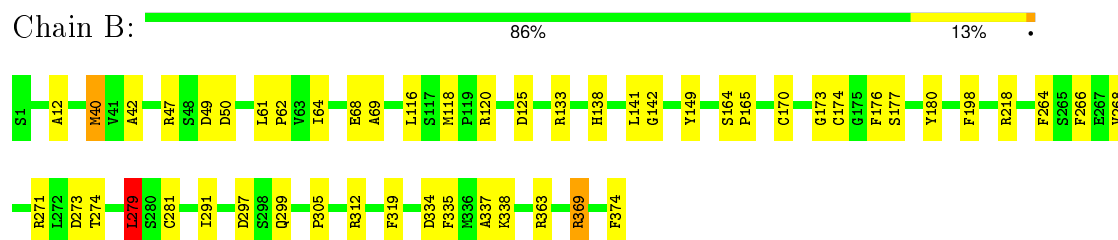
### 3 Residue-property plots

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

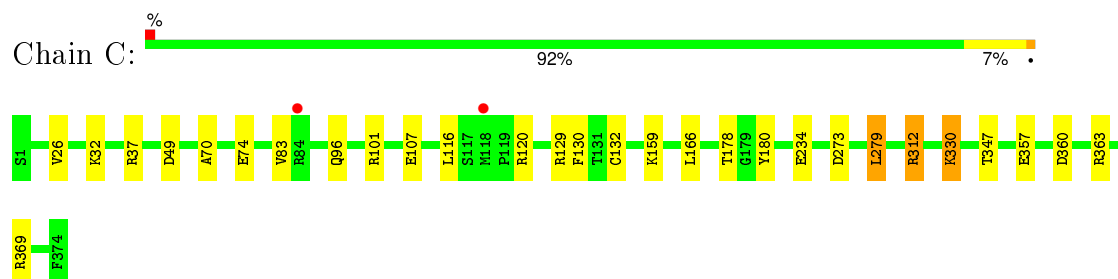
#### • Molecule 1: LIVER ALCOHOL DEHYDROGENASE



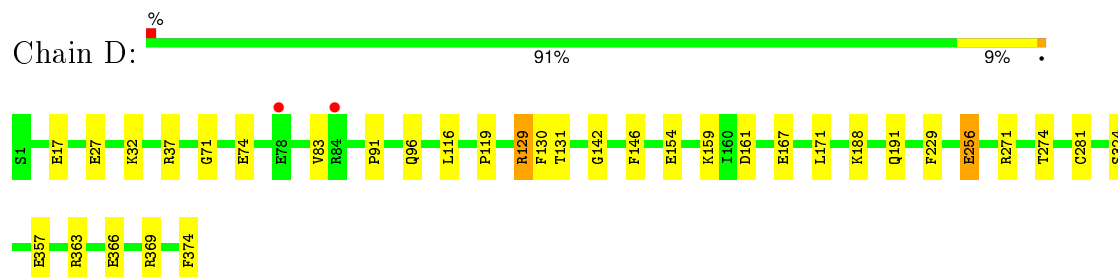
#### • Molecule 1: LIVER ALCOHOL DEHYDROGENASE



#### • Molecule 1: LIVER ALCOHOL DEHYDROGENASE



#### • Molecule 1: LIVER ALCOHOL DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.93 Å   180.20 Å   86.80 Å 90.00°   106.00°   90.00°	Depositor
Resolution (Å)	20.00 – 1.66 19.88 – 1.66	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-1.66) 89.6 (19.88-1.66)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 1.66 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.185 , 0.223 0.176 , 0.206	Depositor DCC
$R_{free}$ test set	1552 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.7	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 155077 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.1322e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: ZN, NAD, SSB

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	0.86	0/2837	1.58	35/3834 (0.9%)
1	B	0.89	2/2837 (0.1%)	1.60	43/3834 (1.1%)
1	C	0.79	0/2837	1.42	14/3834 (0.4%)
1	D	0.84	0/2837	1.50	21/3834 (0.5%)
All	All	0.85	2/11348 (0.0%)	1.53	113/15336 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	SER	CB-OG	5.33	1.49	1.42
1	B	170	CYS	CB-SG	-5.18	1.73	1.81

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	A	264	PHE	CB-CG-CD1	10.32	128.03	120.80
1	B	369	ARG	NE-CZ-NH2	-10.26	115.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ARG	NE-CZ-NH1	10.19	125.40	120.30
1	C	369	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	C	37	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	B	149	TYR	CB-CG-CD2	-9.16	115.50	121.00
1	A	42	ALA	O-C-N	8.46	136.24	122.70
1	A	176	PHE	CB-CG-CD1	-8.45	114.88	120.80
1	D	37	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	D	154	GLU	OE1-CD-OE2	8.42	133.41	123.30
1	A	115	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	A	369	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	B	266	PHE	CB-CG-CD1	-8.26	115.02	120.80
1	B	363	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	319	PHE	CB-CG-CD2	-8.05	115.16	120.80
1	B	49	ASP	CB-CG-OD1	8.03	125.53	118.30
1	D	369	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	B	133	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	B	120	ARG	CA-CB-CG	7.89	130.75	113.40
1	B	125	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	A	264	PHE	CB-CG-CD2	-7.81	115.33	120.80
1	A	40	MET	CG-SD-CE	7.64	112.43	100.20
1	A	84	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	47	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	266	PHE	CB-CG-CD2	7.57	126.10	120.80
1	C	363	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	297	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	335	PHE	CB-CG-CD2	-7.29	115.70	120.80
1	C	273	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	335	PHE	CB-CG-CD1	6.88	125.62	120.80
1	A	146	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	B	279	LEU	CB-CG-CD2	6.78	122.53	111.00
1	B	40	MET	CG-SD-CE	6.72	110.95	100.20
1	C	129	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	148	GLN	O-C-N	-6.57	112.19	122.70
1	B	334	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	266	PHE	CB-CG-CD1	6.51	125.36	120.80
1	D	363	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	335	PHE	CB-CG-CD1	6.45	125.31	120.80
1	B	64	ILE	O-C-N	6.43	132.99	122.70
1	B	291	ILE	O-C-N	6.42	132.97	122.70
1	B	273	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	291	ILE	O-C-N	6.33	132.83	122.70
1	A	149	TYR	CB-CG-CD2	-6.30	117.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	GLN	CG-CD-OE1	6.29	134.17	121.60
1	A	266	PHE	CB-CG-CD2	-6.26	116.42	120.80
1	D	130	PHE	CB-CG-CD1	6.14	125.10	120.80
1	A	161	ASP	CB-CG-OD1	6.14	123.83	118.30
1	C	96	GLN	CG-CD-OE1	6.13	133.87	121.60
1	D	17	GLU	OE1-CD-OE2	6.13	130.65	123.30
1	D	374	PHE	CB-CG-CD2	6.12	125.08	120.80
1	B	125	ASP	CB-CG-OD1	6.06	123.76	118.30
1	A	70	ALA	O-C-N	6.03	133.45	123.20
1	B	68	GLU	CG-CD-OE1	6.03	130.35	118.30
1	B	297	ASP	CB-CG-OD1	6.00	123.69	118.30
1	D	256	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	A	161	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	D	74	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	D	374	PHE	CB-CG-CD1	-5.89	116.67	120.80
1	C	49	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	360	ASP	CB-CG-OD1	5.87	123.59	118.30
1	B	133	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	360	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	D	324	SER	O-C-N	5.72	131.85	122.70
1	B	49	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	315	LYS	O-C-N	5.70	132.88	123.20
1	B	180	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	C	130	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	D	91	PRO	N-CA-CB	5.64	110.07	103.30
1	B	268	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	B	337	ALA	O-C-N	-5.60	113.74	122.70
1	A	342	LEU	O-C-N	-5.57	113.78	122.70
1	D	161	ASP	CB-CG-OD2	5.57	123.32	118.30
1	D	229	PHE	CB-CG-CD1	5.52	124.67	120.80
1	B	174	CYS	CA-CB-SG	-5.52	104.07	114.00
1	D	130	PHE	CB-CG-CD2	-5.51	116.95	120.80
1	B	47	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	A	37	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	154	GLU	CG-CD-OE2	-5.46	107.37	118.30
1	A	84	ARG	CD-NE-CZ	5.46	131.24	123.60
1	B	173	GLY	CA-C-O	-5.44	110.81	120.60
1	B	69	ALA	N-CA-CB	-5.42	102.50	110.10
1	B	120	ARG	CD-NE-CZ	5.41	131.18	123.60
1	D	146	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	A	305	PRO	N-CA-CB	5.41	109.80	103.30
1	C	180	TYR	CB-CG-CD1	-5.40	117.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	PRO	N-CA-CB	5.38	109.76	103.30
1	B	165	PRO	N-CA-CB	5.37	109.74	103.30
1	A	343	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	C	74	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	B	42	ALA	O-C-N	5.32	131.21	122.70
1	B	198	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	176	PHE	CZ-CE2-CD2	-5.29	113.75	120.10
1	C	116	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	317	ALA	O-C-N	5.24	131.08	122.70
1	B	374	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	A	265	SER	N-CA-CB	5.22	118.33	110.50
1	B	176	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	B	264	PHE	CG-CD1-CE1	5.18	126.50	120.80
1	A	311	GLY	CA-C-O	-5.18	111.28	120.60
1	A	125	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	50	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	101	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	A	180	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	D	256	GLU	CB-CG-CD	5.12	128.02	114.20
1	B	138	HIS	O-C-N	5.10	130.85	122.70
1	B	218	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	129	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	30	PRO	N-CA-CB	5.06	109.38	103.30
1	B	176	PHE	CD1-CG-CD2	5.06	124.88	118.30
1	C	312	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	264	PHE	CG-CD1-CE1	5.02	126.32	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	GLY	Mainchain
1	B	12	ALA	Mainchain
1	C	107	GLU	Mainchain
1	D	71	GLY	Mainchain

## 5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2785	0	2848	15	0
1	B	2785	0	2848	9	0
1	C	2785	0	2848	11	0
1	D	2785	0	2848	13	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	44	0	25	1	0
3	B	44	0	25	1	0
3	C	44	0	26	2	0
3	D	44	0	25	1	0
4	A	10	0	16	1	0
4	B	10	0	16	1	0
4	C	10	0	16	1	0
4	D	10	0	16	1	0
5	A	376	0	0	5	0
5	B	437	0	0	3	0
5	C	406	0	0	6	0
5	D	396	0	0	6	0
All	All	12979	0	11557	51	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 2.

All (51) 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:167:GLU:OE2	5:D:548:HOH:O	1.72	1.06
1:D:357:GLU:HG2	5:D:770:HOH:O	1.78	0.82
1:C:120:ARG:HB2	5:C:1041:HOH:O	1.94	0.67
1:D:167:GLU:HG3	5:D:766:HOH:O	1.96	0.66
1:A:230:ALA:O	1:A:234:GLU:HG3	1.99	0.63
1:A:248:LYS:HE2	5:A:745:HOH:O	1.98	0.63
1:A:39:LYS:NZ	5:A:601:HOH:O	2.31	0.62
1:C:234:GLU:HG2	5:C:1125:HOH:O	1.98	0.62
1:C:32:LYS:HE3	5:C:1029:HOH:O	2.01	0.60
1:A:336:MET:HE1	5:A:697:HOH:O	2.06	0.56
1:D:32:LYS:HE3	1:D:129:ARG:CZ	2.35	0.56
1:D:119:PRO:HG3	5:D:769:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:MET:HG2	5:B:611:HOH:O	2.06	0.55
1:A:88:LYS:HD3	1:A:166:LEU:HD21	1.88	0.54
1:C:330:LYS:HG3	5:C:1078:HOH:O	2.06	0.54
1:B:116:LEU:HG	1:B:141:LEU:HD22	1.88	0.54
1:B:279:LEU:HD22	1:B:312:ARG:HD3	1.91	0.52
3:D:377:NAD:C3N	4:D:378:SSB:H22	2.39	0.52
1:A:17:GLU:OE2	1:B:338:LYS:NZ	2.32	0.51
1:C:279:LEU:HD22	1:C:312:ARG:HD3	1.93	0.51
1:C:347:THR:HG21	5:C:1175:HOH:O	2.11	0.50
3:B:377:NAD:C3N	4:B:378:SSB:H22	2.44	0.48
3:A:377:NAD:C3N	4:A:378:SSB:H22	2.43	0.48
3:C:377:NAD:C3N	4:C:378:SSB:H22	2.43	0.48
1:B:61:LEU:HB3	1:B:62:PRO:HA	1.95	0.48
1:A:138:HIS:HE1	5:A:730:HOH:O	1.96	0.47
1:C:26:VAL:HG12	1:C:132:CYS:HB2	1.96	0.47
1:C:178:THR:HG21	3:C:377:NAD:C4N	2.45	0.47
1:A:199:GLY:O	1:A:204:GLY:HA3	2.15	0.46
1:D:167:GLU:H	1:D:167:GLU:CD	2.19	0.46
1:D:366:GLU:O	1:D:366:GLU:HG2	2.15	0.46
1:A:248:LYS:HB2	1:A:249:PRO:HD2	1.98	0.45
1:C:83:VAL:HG12	1:C:159:LYS:HB2	1.98	0.45
1:D:271:ARG:HB2	1:D:274:THR:OG1	2.17	0.45
1:A:68:GLU:OE2	1:A:174:CYS:HB3	2.17	0.45
1:B:299:GLN:NE2	5:B:728:HOH:O	2.50	0.44
1:C:357:GLU:HG3	5:C:1024:HOH:O	2.17	0.44
1:B:142:GLY:HA2	5:B:618:HOH:O	2.18	0.43
1:A:350:LEU:O	1:A:372:LEU:HA	2.20	0.42
1:A:116:LEU:HG	1:A:141:LEU:HD22	2.00	0.42
1:A:350:LEU:HB3	1:A:351:PRO:HD2	2.02	0.42
1:B:369:ARG:HH11	1:B:369:ARG:HD3	1.71	0.42
1:C:70:ALA:HB1	1:C:166:LEU:HD22	2.01	0.42
1:D:142:GLY:HA2	5:D:617:HOH:O	2.20	0.41
1:A:142:GLY:HA2	5:A:672:HOH:O	2.21	0.41
1:A:56:THR:HG23	1:A:296:PRO:HA	2.03	0.41
1:D:171:LEU:HA	1:D:171:LEU:HD23	1.91	0.41
1:D:83:VAL:HG12	1:D:159:LYS:HB2	2.02	0.41
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.21	0.41
1:D:27:GLU:HB2	1:D:131:THR:OG1	2.21	0.40
1:D:188:LYS:HD2	5:D:695:HOH:O	2.22	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	372/374 (100%)	360 (97%)	12 (3%)	0	100	100
1	B	372/374 (100%)	360 (97%)	12 (3%)	0	100	100
1	C	372/374 (100%)	361 (97%)	11 (3%)	0	100	100
1	D	372/374 (100%)	361 (97%)	11 (3%)	0	100	100
All	All	1488/1496 (100%)	1442 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/308 (100%)	306 (99%)	2 (1%)	90	81
1	B	308/308 (100%)	304 (99%)	4 (1%)	76	57
1	C	308/308 (100%)	306 (99%)	2 (1%)	90	81
1	D	308/308 (100%)	304 (99%)	4 (1%)	76	57
All	All	1232/1232 (100%)	1220 (99%)	12 (1%)	82	68

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	251	GLN

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Mol	Chain	Res	Type
1	B	40	MET
1	B	164	SER
1	B	279	LEU
1	B	281	CYS
1	C	279	LEU
1	C	330	LYS
1	D	116	LEU
1	D	191	GLN
1	D	256	GLU
1	D	281	CYS

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

Mol	Chain	Res	Type
1	A	259	ASN
1	B	138	HIS
1	B	299	GLN
1	D	300	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	$\# Z  > 2$
3	NAD	A	377	-	38,48,48	2.15	11 (28%)	47,73,73	3.00	15 (31%)
4	SSB	A	378	2	9,10,10	1.06	0	9,12,12	1.37	2 (22%)
3	NAD	B	377	-	38,48,48	2.04	12 (31%)	47,73,73	3.40	17 (36%)
4	SSB	B	378	2	9,10,10	1.18	1 (11%)	9,12,12	1.28	2 (22%)
3	NAD	C	377	-	38,48,48	1.94	13 (34%)	47,73,73	2.90	14 (29%)
4	SSB	C	378	2	9,10,10	0.94	0	9,12,12	0.95	0
3	NAD	D	377	-	38,48,48	2.00	12 (31%)	47,73,73	3.34	16 (34%)
4	SSB	D	378	2	9,10,10	0.84	0	9,12,12	1.27	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
3	NAD	A	377	-	-	0/22/62/62	0/5/5/5
4	SSB	A	378	2	-	0/4/13/13	0/1/1/1
3	NAD	B	377	-	-	0/22/62/62	0/5/5/5
4	SSB	B	378	2	-	0/4/13/13	0/1/1/1
3	NAD	C	377	-	-	0/22/62/62	0/5/5/5
4	SSB	C	378	2	-	0/4/13/13	0/1/1/1
3	NAD	D	377	-	-	0/22/62/62	0/5/5/5
4	SSB	D	378	2	-	0/4/13/13	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C2N-C3N	-3.90	1.33	1.39
3	B	377	NAD	O2B-C2B	-3.54	1.34	1.43
3	A	377	NAD	O2B-C2B	-3.44	1.34	1.43
3	D	377	NAD	O2D-C2D	-2.80	1.36	1.43
3	A	377	NAD	C2N-C3N	-2.68	1.34	1.39
3	D	377	NAD	C2N-C3N	-2.64	1.34	1.39
3	C	377	NAD	O2B-C2B	-2.55	1.36	1.43
3	A	377	NAD	C6N-C5N	-2.50	1.33	1.38
3	C	377	NAD	PN-O2N	-2.46	1.44	1.54
3	D	377	NAD	PN-O2N	-2.33	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	377	NAD	C2N-C3N	-2.32	1.35	1.39
3	C	377	NAD	O2D-C2D	-2.27	1.37	1.43
3	D	377	NAD	O2B-C2B	-2.23	1.37	1.43
4	B	378	SSB	O6-S1	-2.02	1.43	1.50
3	B	377	NAD	C6N-N1N	2.03	1.40	1.35
3	C	377	NAD	O3B-C3B	2.03	1.47	1.43
3	B	377	NAD	O3B-C3B	2.03	1.47	1.43
3	C	377	NAD	C7N-N7N	2.05	1.37	1.33
3	A	377	NAD	O4B-C4B	2.11	1.49	1.45
3	D	377	NAD	O4B-C4B	2.11	1.49	1.45
3	B	377	NAD	C3D-C4D	2.14	1.58	1.53
3	B	377	NAD	O4D-C4D	2.18	1.50	1.45
3	D	377	NAD	C5N-C4N	2.25	1.43	1.38
3	B	377	NAD	C3N-C7N	2.27	1.54	1.50
3	B	377	NAD	O4D-C1D	2.28	1.44	1.41
3	B	377	NAD	O4B-C4B	2.36	1.50	1.45
3	C	377	NAD	C4A-N3A	2.38	1.39	1.35
3	D	377	NAD	C7N-N7N	2.39	1.37	1.33
3	C	377	NAD	O4B-C4B	2.48	1.50	1.45
3	D	377	NAD	O4D-C1D	2.49	1.44	1.41
3	A	377	NAD	C6N-N1N	2.55	1.42	1.35
3	A	377	NAD	C4A-N3A	2.56	1.39	1.35
3	C	377	NAD	C4N-C3N	2.57	1.43	1.39
3	C	377	NAD	O4D-C1D	2.90	1.44	1.41
3	D	377	NAD	C4N-C3N	3.04	1.44	1.39
3	C	377	NAD	C3N-C7N	3.25	1.55	1.50
3	D	377	NAD	C3N-C7N	3.43	1.55	1.50
3	B	377	NAD	C4N-C3N	3.43	1.45	1.39
3	A	377	NAD	O3B-C3B	3.44	1.51	1.43
3	C	377	NAD	O4D-C4D	3.59	1.53	1.45
3	D	377	NAD	O4D-C4D	3.63	1.53	1.45
3	A	377	NAD	C4N-C3N	3.77	1.45	1.39
3	A	377	NAD	C7N-N7N	4.67	1.42	1.33
3	A	377	NAD	C2A-N3A	5.26	1.41	1.32
3	B	377	NAD	C7N-N7N	5.35	1.43	1.33
3	C	377	NAD	C2A-N3A	5.41	1.41	1.32
3	B	377	NAD	C2A-N3A	5.50	1.41	1.32
3	A	377	NAD	O4D-C1D	5.58	1.48	1.41
3	D	377	NAD	C2A-N3A	6.35	1.43	1.32

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	N3A-C2A-N1A	-13.06	118.89	128.89
3	B	377	NAD	N3A-C2A-N1A	-12.12	119.61	128.89
3	A	377	NAD	N3A-C2A-N1A	-9.91	121.31	128.89
3	C	377	NAD	N3A-C2A-N1A	-9.68	121.48	128.89
3	D	377	NAD	C5N-C4N-C3N	-7.29	111.17	120.33
3	B	377	NAD	C5N-C4N-C3N	-7.11	111.39	120.33
3	A	377	NAD	C5N-C4N-C3N	-6.57	112.08	120.33
3	C	377	NAD	C4B-O4B-C1B	-6.48	102.60	109.72
3	A	377	NAD	C3N-C7N-N7N	-5.63	111.65	117.82
3	C	377	NAD	C5N-C4N-C3N	-5.53	113.38	120.33
3	D	377	NAD	C4B-O4B-C1B	-5.42	103.77	109.72
3	C	377	NAD	C3N-C2N-N1N	-5.30	114.25	120.36
3	B	377	NAD	C3N-C7N-N7N	-5.23	112.09	117.82
3	C	377	NAD	O4D-C1D-N1N	-5.10	102.53	108.13
3	D	377	NAD	O4D-C1D-N1N	-4.79	102.86	108.13
3	D	377	NAD	C3N-C2N-N1N	-4.61	115.05	120.36
3	B	377	NAD	C4B-O4B-C1B	-4.02	105.30	109.72
3	A	377	NAD	C4B-O4B-C1B	-3.47	105.91	109.72
3	A	377	NAD	C1B-N9A-C4A	-3.22	122.09	126.94
3	B	377	NAD	O7N-C7N-N7N	-3.09	118.25	122.59
3	D	377	NAD	O4B-C1B-N9A	-3.03	101.77	108.10
3	C	377	NAD	O4B-C1B-N9A	-2.83	102.17	108.10
3	A	377	NAD	C2B-C1B-N9A	-2.68	110.19	114.29
3	D	377	NAD	C2B-C1B-N9A	-2.52	110.44	114.29
4	A	378	SSB	C2-C3-C7	-2.47	107.63	115.50
3	D	377	NAD	O4D-C4D-C3D	-2.23	100.65	105.15
4	A	378	SSB	C7-C3-C4	-2.22	106.96	115.32
3	D	377	NAD	C5N-C6N-N1N	-2.21	116.64	120.47
3	B	377	NAD	C4N-C3N-C7N	-2.19	115.29	121.09
3	C	377	NAD	C2B-C1B-N9A	-2.19	110.94	114.29
4	B	378	SSB	C2-C3-C7	-2.14	108.69	115.50
4	B	378	SSB	C7-C3-C4	-2.12	107.35	115.32
3	C	377	NAD	O5D-PN-O1N	-2.04	101.71	109.62
3	B	377	NAD	O2A-PA-O5B	-2.03	98.23	108.46
3	B	377	NAD	C5N-C6N-N1N	-2.01	116.99	120.47
3	D	377	NAD	O3D-C3D-C4D	2.08	117.28	111.05
3	C	377	NAD	N6A-C6A-N1A	2.15	123.82	119.20
3	C	377	NAD	C6N-C5N-C4N	2.23	122.81	119.44
3	B	377	NAD	O2B-C2B-C3B	2.32	119.37	111.83
3	A	377	NAD	C2D-C3D-C4D	2.54	107.82	102.61
3	C	377	NAD	C2B-C3B-C4B	2.58	107.91	102.61
3	B	377	NAD	C2D-C3D-C4D	2.59	107.93	102.61
3	A	377	NAD	N6A-C6A-N1A	2.61	124.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	NAD	O2A-PA-O1A	2.66	126.94	112.53
3	D	377	NAD	C2B-C3B-C4B	2.74	108.25	102.61
3	A	377	NAD	O2B-C2B-C3B	2.76	120.80	111.83
3	B	377	NAD	N6A-C6A-N1A	2.93	125.49	119.20
3	D	377	NAD	N6A-C6A-N1A	3.02	125.68	119.20
3	D	377	NAD	O2A-PA-O1A	3.31	130.47	112.53
3	D	377	NAD	C6N-C5N-C4N	3.39	124.56	119.44
3	A	377	NAD	C2B-C3B-C4B	3.50	109.80	102.61
3	B	377	NAD	C2B-C3B-C4B	3.77	110.37	102.61
3	A	377	NAD	PN-O3-PA	3.94	143.79	132.73
3	B	377	NAD	C6N-C5N-C4N	4.38	126.06	119.44
3	B	377	NAD	PN-O3-PA	4.43	145.16	132.73
3	A	377	NAD	C6N-C5N-C4N	4.54	126.30	119.44
3	A	377	NAD	C2N-C3N-C4N	5.29	124.18	118.29
3	C	377	NAD	C2A-N1A-C6A	6.10	129.66	118.77
3	B	377	NAD	C2N-C3N-C4N	6.30	125.30	118.29
3	A	377	NAD	C2A-N1A-C6A	6.45	130.29	118.77
3	B	377	NAD	C2A-N1A-C6A	6.52	130.43	118.77
3	A	377	NAD	O7N-C7N-C3N	6.54	126.73	119.59
3	C	377	NAD	C2N-C3N-C4N	7.31	126.43	118.29
3	D	377	NAD	C2A-N1A-C6A	7.57	132.29	118.77
3	D	377	NAD	C2N-C3N-C4N	8.06	127.27	118.29
3	B	377	NAD	O7N-C7N-C3N	9.19	129.62	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NAD	1	0
4	A	378	SSB	1	0
3	B	377	NAD	1	0
4	B	378	SSB	1	0
3	C	377	NAD	2	0
4	C	378	SSB	1	0
3	D	377	NAD	1	0
4	D	378	SSB	1	0

## 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	374/374 (100%)	-0.18	0 <a href="#">100</a> <a href="#">100</a>	6, 12, 23, 33	0
1	B	374/374 (100%)	-0.16	0 <a href="#">100</a> <a href="#">100</a>	5, 11, 21, 31	0
1	C	374/374 (100%)	0.00	2 (0%) <a href="#">91</a> <a href="#">92</a>	7, 13, 23, 33	0
1	D	374/374 (100%)	-0.15	2 (0%) <a href="#">91</a> <a href="#">92</a>	6, 13, 23, 35	0
All	All	1496/1496 (100%)	-0.12	4 (0%) <a href="#">94</a> <a href="#">94</a>	5, 12, 23, 35	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	ARG	3.4
1	C	118	MET	2.6
1	D	84	ARG	2.5
1	D	78	GLU	2.4

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	SSB	C	378	10/10	0.92	0.14	4.49	12,15,18,20	0
4	SSB	D	378	10/10	0.96	0.11	1.75	14,16,20,21	0
4	SSB	A	378	10/10	0.97	0.10	1.00	5,13,17,19	0
4	SSB	B	378	10/10	0.96	0.11	0.96	6,13,16,18	0
3	NAD	A	377	44/44	0.97	0.07	-0.13	3,12,17,19	0
3	NAD	C	377	44/44	0.96	0.08	-0.48	7,11,17,21	0
3	NAD	B	377	44/44	0.98	0.06	-0.88	4,9,14,18	0
3	NAD	D	377	44/44	0.98	0.06	-0.99	4,10,13,15	0
2	ZN	A	376	1/1	0.99	0.03	-1.43	9,9,9,9	0
2	ZN	B	376	1/1	0.99	0.04	-1.60	11,11,11,11	0
2	ZN	C	376	1/1	0.99	0.03	-1.67	10,10,10,10	0
2	ZN	D	376	1/1	0.99	0.03	-2.45	11,11,11,11	0
2	ZN	A	375	1/1	0.99	0.03	-2.53	10,10,10,10	0
2	ZN	C	375	1/1	0.99	0.04	-2.80	12,12,12,12	0
2	ZN	B	375	1/1	0.99	0.04	-3.35	10,10,10,10	0
2	ZN	D	375	1/1	0.99	0.03	-4.34	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.