



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1E6W  
Title : RAT BRAIN 3-HYDROXYACYL-COA DEHYDROGENASE BINARY  
COMPLEX WITH NADH AND ESTRADIOL  
Authors : Read, J.A.; Powell, A.J.; Brady, R.L.  
Deposited on : 2000-08-23  
Resolution : 1.70 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

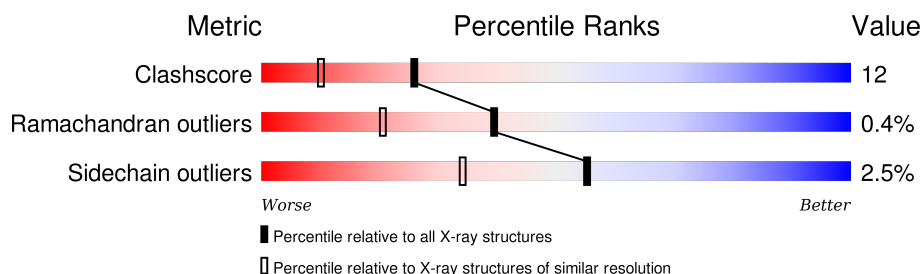
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	
1	D	260	

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
3	EST	L	350	X	-	X	-

## 2 Entry composition [i](#)

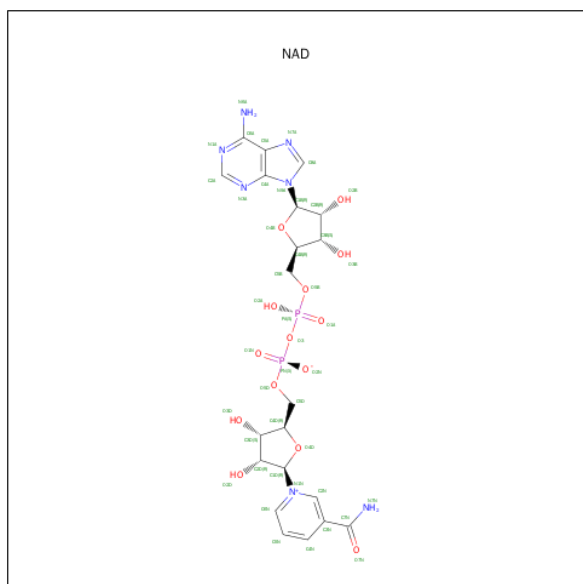
There are 4 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SHORT CHAIN 3-HYDROXYACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	8	0
			1841	1160	323	351	7			
1	B	247	Total	C	N	O	S	0	11	0
			1848	1167	328	347	6			
1	C	248	Total	C	N	O	S	0	5	0
			1820	1147	324	342	7			
1	D	255	Total	C	N	O	S	0	2	0
			1856	1172	329	349	6			

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



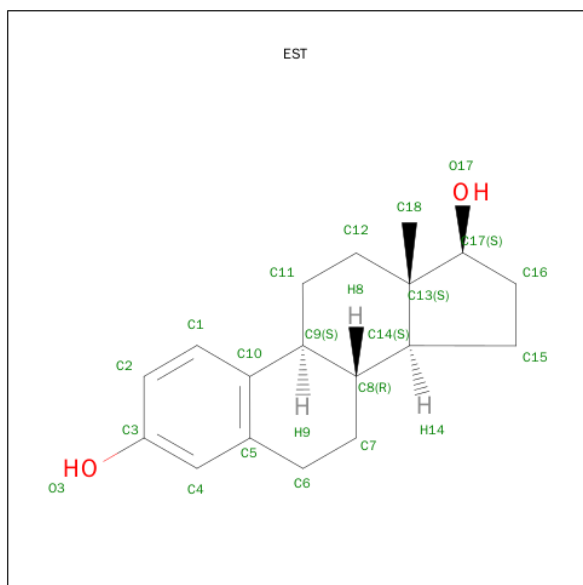
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula:  $C_{18}H_{24}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is water.

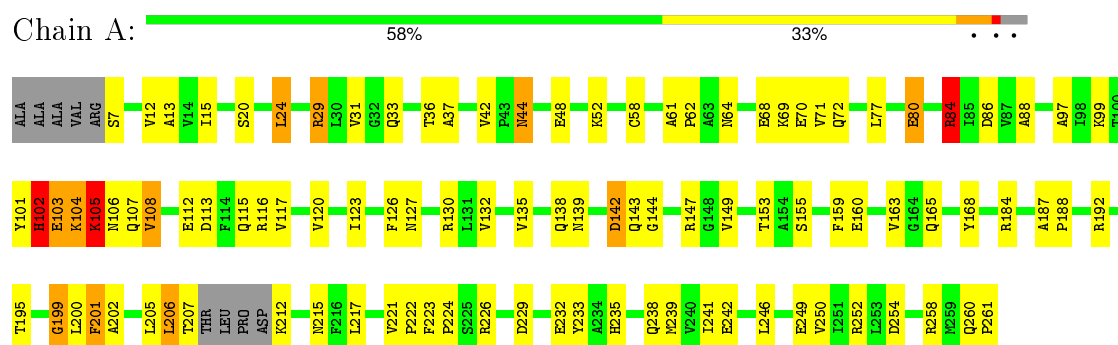
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	128	Total	O	0	0
			128	128		
4	C	143	Total	O	0	0
			143	143		
4	D	128	Total	O	0	0
			128	128		

### 3 Residue-property plots

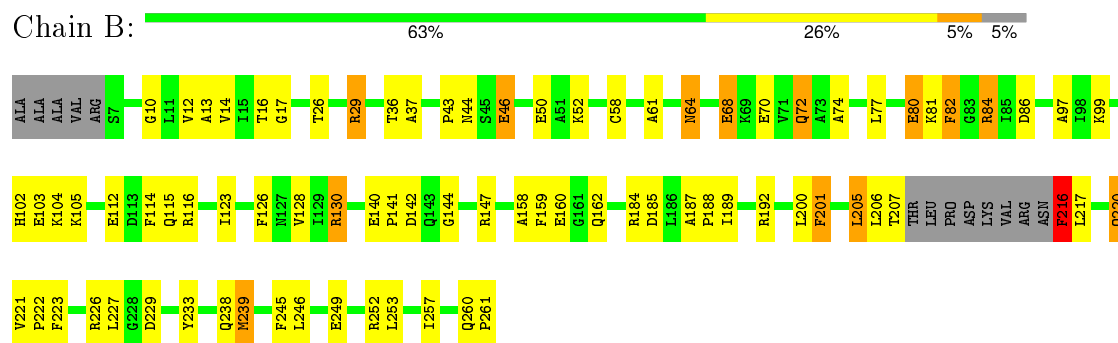
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

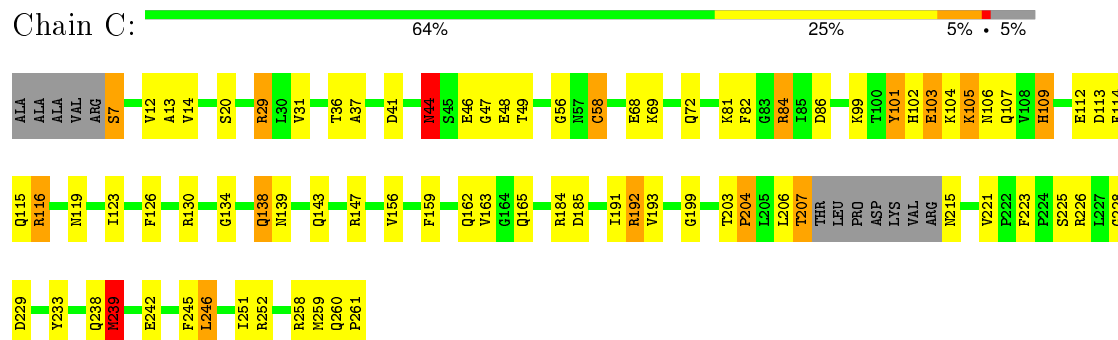
#### • Molecule 1: SHORT CHAIN 3-HYDROXYACYL-COA DEHYDROGENASE



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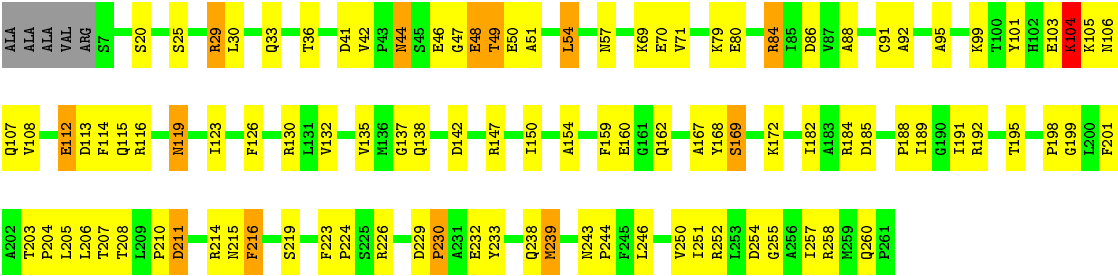
● Molecule 1: SHORT CHAIN 3-HYDROXYACYL-COA DEHYDROGENASE

Chain D: 

58%

34%

5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.60 Å   67.43 Å   67.50 Å 65.22°   73.27°   75.67°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	94.4 (30.00-1.70)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.184 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: EST, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.45	9/1906 (0.5%)	2.31	82/2589 (3.2%)
1	B	1.35	3/1928 (0.2%)	2.19	69/2612 (2.6%)
1	C	1.54	8/1869 (0.4%)	2.31	83/2534 (3.3%)
1	D	1.42	9/1895 (0.5%)	2.31	75/2574 (2.9%)
All	All	1.44	29/7598 (0.4%)	2.28	309/10309 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	10
1	C	0	10
1	D	0	10
All	All	0	39

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	GLU	CD-OE2	7.19	1.33	1.25
1	D	25	SER	CA-CB	6.47	1.62	1.52
1	D	255	GLY	N-CA	6.32	1.55	1.46
1	A	101	TYR	CE1-CZ	-6.12	1.30	1.38
1	A	199	GLY	CA-C	6.10	1.61	1.51
1	A	155	SER	CA-CB	6.09	1.62	1.52
1	A	20	SER	CA-CB	6.03	1.61	1.52
1	A	70	GLU	CD-OE2	5.99	1.32	1.25
1	A	112	GLU	CD-OE2	5.91	1.32	1.25
1	C	48	GLU	CD-OE1	5.88	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	PRO	N-CD	5.84	1.56	1.47
1	C	112	GLU	CA-CB	5.80	1.66	1.53
1	C	261	PRO	N-CD	5.80	1.55	1.47
1	C	252	ARG	CZ-NH2	5.80	1.40	1.33
1	A	70	GLU	CD-OE1	-5.80	1.19	1.25
1	C	20	SER	CA-CB	5.79	1.61	1.52
1	C	225	SER	CB-OG	5.73	1.49	1.42
1	D	184	ARG	NE-CZ	5.67	1.40	1.33
1	C	130	ARG	CZ-NH2	5.66	1.40	1.33
1	B	126	PHE	CE1-CZ	5.59	1.48	1.37
1	D	169	SER	CA-CB	5.44	1.61	1.52
1	A	29	ARG	CZ-NH2	5.44	1.40	1.33
1	B	261	PRO	N-CD	5.37	1.55	1.47
1	D	50	GLU	C-O	5.31	1.33	1.23
1	D	252	ARG	CD-NE	5.25	1.55	1.46
1	D	252	ARG	CZ-NH2	5.24	1.39	1.33
1	C	31	VAL	N-CA	5.22	1.56	1.46
1	B	126	PHE	CG-CD2	5.07	1.46	1.38
1	D	226	ARG	CZ-NH1	5.06	1.39	1.33

All (309) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	CD-NE-CZ	26.25	160.34	123.60
1	D	29	ARG	NE-CZ-NH1	21.82	131.21	120.30
1	A	116	ARG	NE-CZ-NH2	-21.48	109.56	120.30
1	D	252	ARG	NE-CZ-NH1	21.32	130.96	120.30
1	D	226	ARG	NE-CZ-NH2	-20.07	110.27	120.30
1	B	84[A]	ARG	CD-NE-CZ	19.74	151.24	123.60
1	B	84[B]	ARG	CD-NE-CZ	19.74	151.24	123.60
1	C	130	ARG	NE-CZ-NH2	-19.14	110.73	120.30
1	C	116	ARG	CD-NE-CZ	18.66	149.73	123.60
1	D	226	ARG	NE-CZ-NH1	18.21	129.41	120.30
1	D	29	ARG	NE-CZ-NH2	-15.88	112.36	120.30
1	D	184	ARG	NE-CZ-NH1	-15.86	112.37	120.30
1	A	226	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	C	84[A]	ARG	NE-CZ-NH2	14.11	127.35	120.30
1	C	84[B]	ARG	NE-CZ-NH2	14.11	127.35	120.30
1	D	84	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	B	84[A]	ARG	NE-CZ-NH2	13.88	127.24	120.30
1	B	84[B]	ARG	NE-CZ-NH2	13.88	127.24	120.30
1	B	29	ARG	NE-CZ-NH2	-13.13	113.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	A	258	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	D	41	ASP	CB-CG-OD1	12.47	129.52	118.30
1	D	239	MET	CG-SD-CE	12.44	120.11	100.20
1	A	229	ASP	CB-CG-OD1	12.44	129.50	118.30
1	B	229	ASP	CB-CG-OD1	12.09	129.18	118.30
1	C	239[A]	MET	CG-SD-CE	12.07	119.51	100.20
1	C	239[B]	MET	CG-SD-CE	12.07	119.51	100.20
1	C	84[A]	ARG	CD-NE-CZ	11.72	140.01	123.60
1	C	84[B]	ARG	CD-NE-CZ	11.72	140.01	123.60
1	D	192	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	D	84	ARG	NE-CZ-NH2	11.61	126.11	120.30
1	A	116	ARG	NH1-CZ-NH2	11.21	131.73	119.40
1	C	48	GLU	OE1-CD-OE2	11.17	136.71	123.30
1	B	252	ARG	NE-CZ-NH2	11.12	125.86	120.30
1	A	192	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	B	29	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	29	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	B	205	LEU	CA-CB-CG	10.69	139.89	115.30
1	D	113	ASP	CB-CG-OD2	10.21	127.49	118.30
1	C	258	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	A	226	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	B	50	GLU	OE1-CD-OE2	-10.06	111.23	123.30
1	A	130	ARG	NE-CZ-NH2	-10.05	115.28	120.30
1	D	113	ASP	CB-CG-OD1	-9.88	109.41	118.30
1	D	159	PHE	CB-CG-CD1	-9.68	114.03	120.80
1	C	44	ASN	CB-CG-OD1	9.55	140.71	121.60
1	A	252	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	C	233	TYR	CG-CD2-CE2	-9.48	113.72	121.30
1	C	252	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	147	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	A	101	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	A	101	TYR	OH-CZ-CE2	-9.23	95.17	120.10
1	D	201	PHE	CB-CG-CD2	-9.14	114.40	120.80
1	C	147	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	233	TYR	CB-CG-CD2	-9.09	115.54	121.00
1	B	46	GLU	OE1-CD-OE2	-9.09	112.39	123.30
1	B	159	PHE	CB-CG-CD1	-8.87	114.59	120.80
1	C	245	PHE	CB-CG-CD2	8.72	126.90	120.80
1	B	130	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	29	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	114	PHE	CB-CG-CD2	-8.65	114.74	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	48[A]	GLU	OE1-CD-OE2	-8.62	112.96	123.30
1	A	48[B]	GLU	OE1-CD-OE2	-8.62	112.96	123.30
1	A	70	GLU	OE1-CD-OE2	-8.54	113.05	123.30
1	A	101	TYR	CE1-CZ-OH	8.52	143.10	120.10
1	D	252	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	D	107	GLN	CA-CB-CG	8.43	131.94	113.40
1	C	44	ASN	CA-CB-CG	8.42	131.93	113.40
1	D	116	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	C	126	PHE	CG-CD2-CE2	-8.18	111.81	120.80
1	D	114	PHE	CB-CG-CD1	-8.16	115.08	120.80
1	C	103	GLU	OE1-CD-OE2	-8.13	113.55	123.30
1	D	239	MET	CA-CB-CG	8.13	127.12	113.30
1	C	41	ASP	CB-CG-OD1	8.08	125.57	118.30
1	D	130	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	B	216	PHE	CB-CG-CD2	-8.01	115.19	120.80
1	C	223	PHE	CB-CG-CD2	8.00	126.40	120.80
1	B	245	PHE	CB-CG-CD1	7.99	126.39	120.80
1	C	242	GLU	OE1-CD-OE2	-7.96	113.74	123.30
1	B	184	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	C	101	TYR	CB-CG-CD2	-7.81	116.32	121.00
1	C	233	TYR	CD1-CE1-CZ	-7.68	112.88	119.80
1	A	233	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	229	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	D	147	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	D	184	ARG	NH1-CZ-NH2	7.61	127.77	119.40
1	A	101	TYR	CG-CD2-CE2	-7.60	115.22	121.30
1	C	29	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	44	ASN	CB-CG-ND2	-7.57	98.54	116.70
1	A	202	ALA	N-CA-CB	-7.56	99.52	110.10
1	D	126	PHE	CB-CG-CD1	-7.56	115.51	120.80
1	A	201	PHE	CB-CG-CD2	7.50	126.05	120.80
1	A	168	TYR	CB-CG-CD1	-7.48	116.51	121.00
1	A	184	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	127	ASN	OD1-CG-ND2	7.48	139.10	121.90
1	D	49	THR	CA-CB-OG1	-7.46	93.33	109.00
1	A	142	ASP	CB-CG-OD2	-7.42	111.63	118.30
1	C	130	ARG	NH1-CZ-NH2	7.41	127.55	119.40
1	B	216	PHE	CB-CG-CD1	7.40	125.98	120.80
1	A	160	GLU	OE1-CD-OE2	7.39	132.17	123.30
1	C	226	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	252	ARG	NE-CZ-NH2	7.29	123.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	PHE	CB-CG-CD2	-7.28	115.70	120.80
1	B	160	GLU	OE1-CD-OE2	7.25	132.00	123.30
1	D	168	TYR	CB-CG-CD1	7.24	125.34	121.00
1	B	229	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	D	142	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	C	72	GLN	CG-CD-OE1	-7.06	107.47	121.60
1	B	29	ARG	CD-NE-CZ	-7.05	113.72	123.60
1	D	201	PHE	CB-CG-CD1	7.04	125.72	120.80
1	C	72	GLN	CB-CG-CD	7.01	129.83	111.60
1	A	159	PHE	CB-CG-CD1	-6.99	115.91	120.80
1	B	246	LEU	CA-CB-CG	6.99	131.37	115.30
1	C	229	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	C	105	LYS	CD-CE-NZ	6.92	127.61	111.70
1	C	126	PHE	CB-CG-CD1	-6.90	115.97	120.80
1	D	70	GLU	OE1-CD-OE2	-6.89	115.03	123.30
1	B	226	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	191	ILE	O-C-N	6.83	133.62	122.70
1	C	159	PHE	CG-CD2-CE2	-6.82	113.30	120.80
1	D	233	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	A	226	ARG	CB-CA-C	-6.78	96.83	110.40
1	D	239	MET	CB-CG-SD	6.78	132.74	112.40
1	C	207	THR	N-CA-CB	6.77	123.16	110.30
1	B	70	GLU	CG-CD-OE1	6.73	131.75	118.30
1	B	142	ASP	CB-CG-OD1	6.71	124.33	118.30
1	D	71	VAL	CA-CB-CG2	-6.69	100.87	110.90
1	A	226	ARG	O-C-N	6.69	133.40	122.70
1	A	80	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	B	253	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	D	116	ARG	NH1-CZ-NH2	6.62	126.68	119.40
1	B	140	GLU	CG-CD-OE1	6.60	131.50	118.30
1	D	112	GLU	OE1-CD-OE2	-6.56	115.43	123.30
1	C	48	GLU	CA-CB-CG	-6.56	98.97	113.40
1	B	252	ARG	NH1-CZ-NH2	-6.56	112.19	119.40
1	A	147	ARG	NH1-CZ-NH2	-6.53	112.22	119.40
1	B	103	GLU	OE1-CD-OE2	-6.51	115.49	123.30
1	B	205	LEU	CA-C-O	-6.49	106.47	120.10
1	A	117	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	A	149	VAL	O-C-N	6.49	133.08	122.70
1	D	103	GLU	OE1-CD-OE2	6.45	131.04	123.30
1	D	258	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	160	GLU	CG-CD-OE2	-6.44	105.42	118.30
1	C	72	GLN	CG-CD-NE2	6.43	132.14	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	PHE	O-C-N	-6.43	112.28	123.20
1	D	126	PHE	O-C-N	6.40	132.95	122.70
1	D	150	ILE	O-C-N	6.38	132.92	122.70
1	A	86	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	D	188	PRO	O-C-N	-6.35	112.54	122.70
1	D	191	ILE	O-C-N	6.35	132.85	122.70
1	D	116	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	88	ALA	O-C-N	6.31	132.80	122.70
1	A	112	GLU	CG-CD-OE2	-6.30	105.70	118.30
1	A	77	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	D	229	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	198	PRO	N-CD-CG	-6.28	93.78	103.20
1	D	168	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	C	126	PHE	CZ-CE2-CD2	6.25	127.60	120.10
1	D	30	LEU	CB-CG-CD2	6.23	121.59	111.00
1	C	193	VAL	CA-CB-CG2	6.21	120.22	110.90
1	C	159	PHE	CB-CG-CD2	-6.21	116.45	120.80
1	B	14	VAL	CA-CB-CG2	-6.20	101.61	110.90
1	D	215	ASN	O-C-N	-6.20	112.79	122.70
1	C	184	ARG	NH1-CZ-NH2	6.18	126.19	119.40
1	B	239	MET	CB-CA-C	6.14	122.69	110.40
1	D	54	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	D	252	ARG	NH1-CZ-NH2	-6.13	112.65	119.40
1	D	119	ASN	CB-CG-OD1	6.13	133.86	121.60
1	B	147	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	13	ALA	N-CA-CB	-6.12	101.54	110.10
1	A	113	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	C	20	SER	N-CA-CB	-6.10	101.34	110.50
1	B	97	ALA	N-CA-CB	6.10	118.64	110.10
1	A	42	VAL	CA-CB-CG2	6.09	120.04	110.90
1	D	216	PHE	CB-CG-CD1	6.08	125.06	120.80
1	B	82	PHE	CB-CG-CD2	6.08	125.05	120.80
1	B	130	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	86	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	B	80	GLU	CA-C-O	-6.06	107.37	120.10
1	B	46	GLU	CG-CD-OE2	6.04	130.38	118.30
1	B	84[A]	ARG	NH1-CZ-NH2	-6.01	112.78	119.40
1	B	84[B]	ARG	NH1-CZ-NH2	-6.01	112.78	119.40
1	A	112	GLU	CA-CB-CG	-6.01	100.19	113.40
1	B	192	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	229	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	162	GLN	CG-CD-OE1	-6.00	109.60	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	70	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	A	104	LYS	CA-CB-CG	6.00	126.59	113.40
1	C	159	PHE	CD1-CG-CD2	5.98	126.07	118.30
1	B	72	GLN	CB-CA-C	-5.92	98.55	110.40
1	B	249	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	C	109	HIS	O-C-N	-5.92	113.22	122.70
1	B	80	GLU	CA-C-N	5.92	130.23	117.20
1	A	44	ASN	O-C-N	-5.91	113.24	122.70
1	A	153	THR	CA-CB-CG2	-5.89	104.15	112.40
1	C	215	ASN	CA-CB-CG	5.88	126.34	113.40
1	A	108	VAL	CG1-CB-CG2	-5.87	101.52	110.90
1	A	201	PHE	O-C-N	5.86	132.08	122.70
1	C	260[A]	GLN	CB-CG-CD	5.83	126.76	111.60
1	C	260[B]	GLN	CB-CG-CD	5.83	126.76	111.60
1	D	185	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	24	LEU	O-C-N	-5.83	113.38	122.70
1	C	185	ASP	CB-CG-OD1	5.82	123.53	118.30
1	D	169	SER	O-C-N	-5.81	113.41	122.70
1	D	192	ARG	CD-NE-CZ	5.81	131.73	123.60
1	D	104	LYS	CA-CB-CG	5.80	126.17	113.40
1	B	13	ALA	CB-CA-C	-5.78	101.43	110.10
1	C	130	ARG	CG-CD-NE	-5.77	99.68	111.80
1	A	97	ALA	N-CA-CB	5.76	118.17	110.10
1	B	52	LYS	CD-CE-NZ	5.74	124.91	111.70
1	D	119	ASN	OD1-CG-ND2	-5.74	108.69	121.90
1	C	126	PHE	CD1-CG-CD2	5.74	125.76	118.30
1	B	223	PHE	CB-CG-CD2	5.73	124.81	120.80
1	C	185	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	126	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	A	184	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	84	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	44	ASN	CB-CA-C	5.62	121.65	110.40
1	C	112	GLU	CA-CB-CG	-5.62	101.04	113.40
1	C	14	VAL	CA-CB-CG1	-5.60	102.49	110.90
1	A	205	LEU	N-CA-CB	-5.60	99.20	110.40
1	C	252	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	84[A]	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	C	84[B]	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	D	160	GLU	CG-CD-OE2	-5.60	107.11	118.30
1	D	260	GLN	C-N-CD	5.58	140.12	128.40
1	B	26	THR	CA-CB-CG2	5.58	120.21	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	GLN	CB-CG-CD	5.57	126.09	111.60
1	B	226	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	56	GLY	O-C-N	5.54	131.57	122.70
1	A	233	TYR	CG-CD1-CE1	-5.52	116.88	121.30
1	C	103	GLU	CG-CD-OE2	5.52	129.33	118.30
1	C	233	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	D	192	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	B	114	PHE	CB-CG-CD1	5.47	124.63	120.80
1	D	150	ILE	CA-C-O	-5.45	108.65	120.10
1	D	20	SER	N-CA-CB	-5.43	102.35	110.50
1	A	249	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	A	71	VAL	CA-CB-CG2	-5.41	102.78	110.90
1	D	230	PRO	O-C-N	-5.39	114.07	122.70
1	D	162	GLN	OE1-CD-NE2	5.39	134.29	121.90
1	C	221	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	A	233	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	A	201	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	C	138	GLN	OE1-CD-NE2	-5.33	109.63	121.90
1	A	222	PRO	N-CA-CB	5.32	109.69	103.30
1	D	86	ASP	O-C-N	5.31	131.19	122.70
1	A	68	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	13	ALA	N-CA-CB	-5.28	102.71	110.10
1	D	167	ALA	N-CA-CB	-5.27	102.72	110.10
1	C	163	VAL	CA-CB-CG1	-5.27	103.00	110.90
1	A	242	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	C	259	MET	O-C-N	5.26	131.11	122.70
1	B	68	GLU	CA-CB-CG	-5.25	101.84	113.40
1	A	88	ALA	N-CA-CB	-5.25	102.74	110.10
1	A	254	ASP	N-CA-CB	-5.24	101.16	110.60
1	D	48	GLU	CA-CB-CG	-5.24	101.88	113.40
1	A	163	VAL	CA-CB-CG1	-5.24	103.05	110.90
1	A	102	HIS	O-C-N	-5.23	114.33	122.70
1	C	82	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	C	113	ASP	O-C-N	5.22	131.05	122.70
1	B	201	PHE	CB-CG-CD2	5.22	124.45	120.80
1	B	112[A]	GLU	CB-CG-CD	5.20	128.25	114.20
1	B	112[B]	GLU	CB-CG-CD	5.20	128.25	114.20
1	A	64	ASN	N-CA-CB	-5.18	101.27	110.60
1	D	215	ASN	C-N-CA	5.18	134.65	121.70
1	C	112	GLU	N-CA-CB	-5.18	101.28	110.60
1	C	260[A]	GLN	CA-C-O	5.18	130.97	120.10
1	C	260[B]	GLN	CA-C-O	5.18	130.97	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	232	GLU	CG-CD-OE1	5.16	128.62	118.30
1	C	107	GLN	O-C-N	5.16	130.95	122.70
1	A	15	ILE	O-C-N	5.14	130.93	122.70
1	A	29	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
1	B	140	GLU	OE1-CD-OE2	-5.13	117.15	123.30
1	B	147	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	A	135	VAL	O-C-N	-5.11	114.52	122.70
1	B	43	PRO	O-C-N	-5.11	114.52	122.70
1	B	158	ALA	CB-CA-C	-5.11	102.43	110.10
1	D	44	ASN	CB-CA-C	5.11	120.62	110.40
1	A	31	VAL	O-C-N	-5.11	114.52	123.20
1	A	235	HIS	N-CA-CB	-5.10	101.42	110.60
1	B	223	PHE	CG-CD2-CE2	5.10	126.41	120.80
1	D	46	GLU	CA-CB-CG	5.10	124.62	113.40
1	C	156	VAL	CA-CB-CG1	-5.10	103.25	110.90
1	C	207	THR	CA-CB-OG1	5.10	119.70	109.00
1	D	33	GLN	CG-CD-NE2	-5.10	104.47	116.70
1	B	158	ALA	O-C-N	5.08	130.84	122.70
1	B	77	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	A	168	TYR	CB-CG-CD2	5.07	124.04	121.00
1	B	64	ASN	N-CA-CB	-5.07	101.48	110.60
1	B	74	ALA	N-CA-CB	-5.06	103.01	110.10
1	C	68	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	C	68	GLU	N-CA-CB	-5.06	101.49	110.60
1	D	92	ALA	N-CA-CB	-5.05	103.03	110.10
1	D	132	VAL	CA-CB-CG1	5.05	118.48	110.90
1	C	7	SER	CA-CB-OG	5.05	124.83	111.20
1	A	70	GLU	O-C-N	5.04	130.76	122.70
1	C	192	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	215	ASN	OD1-CG-ND2	-5.03	110.33	121.90
1	B	245	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	B	221	VAL	CA-CB-CG2	5.03	118.44	110.90
1	A	165	GLN	O-C-N	-5.02	114.67	122.70
1	A	241	ILE	N-CA-CB	-5.02	99.25	110.80
1	C	246	LEU	CA-CB-CG	5.02	126.84	115.30
1	D	260	GLN	CA-C-O	5.01	130.62	120.10
1	A	258	ARG	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	HIS	Mainchain
1	A	105	LYS	Mainchain
1	A	120	VAL	Mainchain
1	A	139	ASN	Mainchain
1	A	144	GLY	Mainchain
1	A	199	GLY	Mainchain
1	A	217	LEU	Mainchain
1	A	24	LEU	Mainchain
1	A	7	SER	Mainchain
1	B	10	GLY	Mainchain
1	B	144	GLY	Mainchain
1	B	17	GLY	Mainchain
1	B	189	ILE	Mainchain
1	B	205	LEU	Mainchain
1	B	222	PRO	Mainchain
1	B	61	ALA	Mainchain
1	B	64	ASN	Mainchain
1	B	80	GLU	Mainchain
1	B	81	LYS	Mainchain
1	C	123	ILE	Mainchain
1	C	138	GLN	Mainchain
1	C	143	GLN	Mainchain
1	C	199	GLY	Mainchain
1	C	203	THR	Mainchain
1	C	228	GLY	Mainchain
1	C	251	ILE	Mainchain
1	C	47	GLY	Mainchain
1	C	58	CYS	Mainchain
1	C	81	LYS	Mainchain
1	D	135	VAL	Mainchain
1	D	137	GLY	Mainchain
1	D	169	SER	Mainchain
1	D	199	GLY	Mainchain
1	D	205	LEU	Mainchain
1	D	211	ASP	Mainchain
1	D	42	VAL	Mainchain
1	D	47	GLY	Mainchain
1	D	51	ALA	Mainchain
1	D	91	CYS	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	1841	0	1864	54	2
1	B	1848	0	1916	48	4
1	C	1820	0	1872	58	2
1	D	1856	0	1889	42	6
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
3	L	20	0	21	11	0
4	A	146	0	0	15	1
4	B	128	0	0	12	3
4	C	143	0	0	14	3
4	D	128	0	0	11	1
All	All	8106	0	7666	190	11

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 12.

All (190) 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:239:MET:HG2	4:D:2109:HOH:O	1.63	0.98
1:A:29:ARG:HE	1:A:238[B]:GLN:NE2	1.62	0.95
1:D:29:ARG:HE	1:D:238[B]:GLN:NE2	1.64	0.94
1:D:29:ARG:HH21	1:D:238[B]:GLN:HE22	0.96	0.94
1:D:29:ARG:HE	1:D:238[B]:GLN:HE21	0.94	0.93
1:C:101:TYR:HE2	4:C:2064:HOH:O	1.52	0.91
1:A:239[A]:MET:CG	1:C:239[A]:MET:HG3	2.01	0.91
1:B:141:PRO:CD	4:B:2069:HOH:O	2.19	0.90
1:A:239[A]:MET:HG3	1:C:239[A]:MET:HG3	1.54	0.89
1:B:29:ARG:HH21	1:B:238[B]:GLN:HE22	1.12	0.89
1:D:29:ARG:HH21	1:D:238[B]:GLN:NE2	1.72	0.87
1:C:206:LEU:HD23	3:L:350:EST:H151	1.55	0.87
1:B:29:ARG:NH2	1:B:238[B]:GLN:HE22	1.73	0.86
1:C:29:ARG:HH21	1:C:238[B]:GLN:HE22	1.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ARG:NE	1:D:238[B]:GLN:HE21	1.77	0.82
1:A:103:GLU:OE2	1:B:188:PRO:HB2	1.81	0.81
1:B:29:ARG:HE	1:B:238[B]:GLN:HE21	1.28	0.81
1:C:12:VAL:HG23	1:C:84[A]:ARG:NH1	1.96	0.81
1:A:29:ARG:HE	1:A:238[B]:GLN:HE21	1.24	0.80
1:D:29:ARG:NH2	1:D:238[B]:GLN:HE22	1.78	0.80
1:B:29:ARG:HH21	1:B:238[B]:GLN:NE2	1.80	0.80
1:D:79:LYS:HE3	4:D:2042:HOH:O	1.83	0.79
1:B:141:PRO:CG	4:B:2069:HOH:O	2.30	0.79
1:B:29:ARG:HE	1:B:238[B]:GLN:NE2	1.81	0.78
1:C:29:ARG:HE	1:C:238[B]:GLN:NE2	1.81	0.78
1:B:46:GLU:HG2	4:B:2022:HOH:O	1.82	0.78
1:C:46:GLU:HG3	4:C:2026:HOH:O	1.84	0.77
1:C:101:TYR:CE2	4:C:2064:HOH:O	2.31	0.76
1:A:212:LYS:HA	4:A:2115:HOH:O	1.85	0.76
1:C:29:ARG:HE	1:C:238[B]:GLN:HE21	1.33	0.74
1:A:36[A]:THR:HG23	4:A:2015:HOH:O	1.90	0.71
1:A:239[A]:MET:HG3	1:C:239[A]:MET:CG	2.20	0.71
1:C:99:LYS:HD3	4:D:2093:HOH:O	1.90	0.70
1:D:36:THR:HG23	4:D:2013:HOH:O	1.91	0.70
1:A:106:ASN:HB3	4:A:2067:HOH:O	1.92	0.70
1:A:29:ARG:HH21	1:A:238[B]:GLN:HE22	1.42	0.67
1:C:44:ASN:HB2	4:C:2020:HOH:O	1.94	0.67
1:B:260:GLN:NE2	4:B:2121:HOH:O	2.28	0.66
1:A:29:ARG:NE	1:A:238[B]:GLN:NE2	2.41	0.66
1:B:29:ARG:NE	1:B:238[B]:GLN:HE21	1.94	0.66
1:B:116[A]:ARG:HH11	1:B:116[A]:ARG:HB3	1.60	0.65
1:D:29:ARG:NE	1:D:238[B]:GLN:NE2	2.40	0.65
1:B:29:ARG:NE	1:B:238[B]:GLN:NE2	2.43	0.65
1:B:220:GLN:HB3	4:B:2121:HOH:O	1.96	0.64
1:B:207:THR:HG21	4:B:2090:HOH:O	1.97	0.64
1:A:115[B]:GLN:NE2	1:B:123:ILE:HD13	2.13	0.64
1:A:239[A]:MET:HB2	1:C:239[A]:MET:HG3	1.79	0.64
2:C:301:NAD:O7N	3:L:350:EST:H162	1.98	0.63
1:C:206:LEU:CD2	3:L:350:EST:H151	2.27	0.63
1:B:68:GLU:OE2	1:B:72:GLN:NE2	2.31	0.63
1:A:239[B]:MET:CG	1:C:239[B]:MET:HG3	2.29	0.63
4:C:2101:HOH:O	3:L:350:EST:H112	1.98	0.62
1:C:29:ARG:HH21	1:C:238[B]:GLN:NE2	1.96	0.61
1:B:239:MET:CB	1:D:239:MET:HG3	2.30	0.61
1:A:105:LYS:HD3	1:A:107:GLN:NE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2101:HOH:O	3:L:350:EST:H1	1.99	0.61
1:A:207:THR:HA	4:A:2112:HOH:O	1.99	0.61
1:B:29:ARG:NH2	1:B:238[B]:GLN:NE2	2.44	0.60
1:C:116:ARG:HD3	4:C:2074:HOH:O	2.00	0.60
1:A:33[B]:GLN:HE22	1:A:238[B]:GLN:NE2	1.98	0.60
1:B:104:LYS:HG3	1:B:105:LYS:HD2	1.83	0.60
1:D:105:LYS:HG3	4:D:2054:HOH:O	2.00	0.60
1:B:68:GLU:O	1:B:72:GLN:HG3	2.02	0.59
1:B:260:GLN:HG2	4:B:2122:HOH:O	2.02	0.59
1:C:49:THR:HG23	4:C:2029:HOH:O	2.01	0.59
1:A:239[B]:MET:HG2	1:C:239[B]:MET:CG	2.32	0.59
1:C:165:GLN:HE22	3:L:350:EST:H121	1.67	0.59
1:C:165:GLN:NE2	3:L:350:EST:H121	2.19	0.58
1:C:29:ARG:NH2	1:C:238[B]:GLN:HE22	1.97	0.58
1:C:84[A]:ARG:CZ	1:C:86:ASP:OD2	2.52	0.58
1:B:116[A]:ARG:NH1	1:B:116[A]:ARG:HB3	2.19	0.58
1:A:99:LYS:HD3	4:A:2060:HOH:O	2.03	0.57
1:B:217:LEU:HB2	4:B:2095:HOH:O	2.04	0.57
1:D:69:LYS:HG3	4:D:2037:HOH:O	2.05	0.57
1:C:204:PRO:O	1:C:207:THR:N	2.38	0.56
1:A:142:ASP:HB2	4:A:2086:HOH:O	2.05	0.56
2:C:301:NAD:C7N	3:L:350:EST:H162	2.36	0.56
1:A:239[B]:MET:CG	1:C:239[B]:MET:CG	2.85	0.55
1:A:44:ASN:HB2	4:A:2019:HOH:O	2.06	0.55
1:A:223:PHE:CD1	1:A:224:PRO:HA	2.41	0.55
1:B:216:PHE:N	4:B:2092:HOH:O	2.40	0.55
1:B:200:LEU:HD13	1:B:217:LEU:HB3	1.89	0.54
1:A:108:VAL:HG12	4:A:2069:HOH:O	2.08	0.54
1:A:239[A]:MET:CG	1:C:239[A]:MET:CG	2.79	0.54
1:A:239[B]:MET:HG2	1:C:239[B]:MET:HG3	1.87	0.54
1:C:102:HIS:CD2	1:C:105:LYS:HG3	2.43	0.53
1:A:201:PHE:O	1:A:206:LEU:HD22	2.07	0.53
1:D:29:ARG:NH2	1:D:238[B]:GLN:NE2	2.45	0.53
1:C:36:THR:HG23	4:C:2017:HOH:O	2.08	0.53
1:B:102:HIS:CD2	1:B:104:LYS:HG2	2.44	0.52
1:D:254:ASP:HB2	1:D:257:ILE:HG22	1.91	0.52
1:A:12:VAL:HG23	1:A:84:ARG:NH1	2.23	0.52
1:A:12:VAL:HG23	1:A:84:ARG:HH11	1.74	0.52
1:D:203:THR:HB	1:D:204:PRO:CD	2.40	0.52
1:B:68:GLU:HG2	1:B:72:GLN:HE21	1.74	0.51
1:B:102:HIS:NE2	1:B:104:LYS:HG2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:HG3	4:A:2086:HOH:O	2.10	0.51
1:B:84[A]:ARG:NH1	1:B:86:ASP:OD2	2.43	0.51
1:A:44:ASN:ND2	4:A:2018:HOH:O	2.35	0.51
1:C:115[A]:GLN:OE1	1:D:123[A]:ILE:HD13	2.10	0.51
1:A:29:ARG:NH2	1:A:238[B]:GLN:HE22	2.09	0.51
1:C:103:GLU:O	1:C:106:ASN:N	2.37	0.51
1:D:216:PHE:N	1:D:216:PHE:CD1	2.79	0.51
1:C:29:ARG:NE	1:C:238[B]:GLN:NE2	2.55	0.50
1:C:101:TYR:OH	1:C:106:ASN:ND2	2.41	0.50
1:C:29:ARG:NE	1:C:238[B]:GLN:HE21	2.06	0.50
1:D:216:PHE:O	1:D:219:SER:OG	2.29	0.50
1:C:134:GLY:HA2	4:C:2081:HOH:O	2.11	0.50
1:A:221:VAL:HG21	4:A:2110:HOH:O	2.12	0.50
1:D:95:ALA:HB3	1:D:208:THR:HG21	1.92	0.50
1:B:227:LEU:N	4:B:2100:HOH:O	1.77	0.50
1:A:33[B]:GLN:NE2	1:A:238[B]:GLN:NE2	2.60	0.49
1:A:52:LYS:CD	4:A:2028:HOH:O	2.60	0.49
1:A:187:ALA:N	1:A:188:PRO:HD2	2.26	0.49
1:A:195:THR:HB	1:A:250:VAL:HG22	1.94	0.49
1:D:154:ALA:HA	1:D:172:LYS:HD2	1.94	0.48
1:D:119:ASN:HB3	4:D:2068:HOH:O	2.12	0.48
4:C:2100:HOH:O	3:L:350:EST:H122	2.13	0.48
1:D:36:THR:HG22	1:D:57:ASN:HB3	1.95	0.48
1:A:33[B]:GLN:HE22	1:A:238[B]:GLN:CD	2.17	0.48
1:B:68:GLU:HG3	1:B:130:ARG:NH2	2.28	0.48
1:D:101:TYR:HD1	1:D:108:VAL:HG22	1.78	0.48
1:A:37:ALA:O	1:A:58:CYS:HA	2.13	0.48
1:A:260[B]:GLN:HG2	4:A:2137:HOH:O	2.14	0.48
1:A:44:ASN:CB	4:A:2019:HOH:O	2.61	0.47
1:A:239[A]:MET:SD	1:A:246:LEU:CD2	3.02	0.47
1:B:239:MET:HG3	1:D:239:MET:HG3	1.96	0.47
1:A:12:VAL:HG22	1:A:36[A]:THR:OG1	2.15	0.47
1:C:239[B]:MET:SD	1:C:246:LEU:CD2	3.03	0.47
1:C:12:VAL:HG23	1:C:84[A]:ARG:HH12	1.76	0.47
1:B:201:PHE:O	1:B:206:LEU:HD12	2.15	0.46
1:A:187:ALA:N	1:A:188:PRO:CD	2.78	0.46
1:A:239[B]:MET:HG2	1:C:239[B]:MET:HG2	1.96	0.46
1:C:103:GLU:O	1:C:104:LYS:C	2.51	0.46
1:D:239:MET:SD	4:D:2109:HOH:O	2.61	0.46
1:B:36[B]:THR:HG21	1:B:82:PHE:CE1	2.50	0.46
1:D:84:ARG:HH11	1:D:84:ARG:HD2	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ASN:CB	4:D:2068:HOH:O	2.64	0.46
1:B:217:LEU:N	4:B:2095:HOH:O	2.49	0.46
1:D:223:PHE:CD1	1:D:224:PRO:HA	2.51	0.45
1:C:69:LYS:HE3	4:C:2045:HOH:O	2.16	0.45
1:A:105:LYS:HE2	1:A:107:GLN:NE2	2.31	0.45
1:D:79:LYS:NZ	1:D:138:GLN:OE1	2.35	0.45
1:C:105:LYS:O	1:C:106:ASN:C	2.54	0.45
1:B:68:GLU:HG2	1:B:72:GLN:NE2	2.30	0.45
1:D:246:LEU:HD21	1:D:251:ILE:HD11	1.99	0.45
1:A:29:ARG:NE	1:A:238[B]:GLN:HE21	2.04	0.45
1:C:192:ARG:HD2	1:C:246:LEU:O	2.17	0.45
1:A:138:GLN:OE1	1:A:138:GLN:HA	2.15	0.45
1:C:84[B]:ARG:NH2	1:C:139:ASN:HB3	2.32	0.44
1:A:102:HIS:NE2	1:A:104:LYS:HE2	2.33	0.44
1:D:182:ILE:HG21	1:D:182:ILE:HD13	1.78	0.44
1:D:101:TYR:CD1	1:D:108:VAL:HG22	2.52	0.44
1:D:195:THR:HB	1:D:250:VAL:HG22	1.99	0.44
4:C:2107:HOH:O	1:D:99:LYS:HD3	2.18	0.44
1:D:195:THR:O	1:D:250:VAL:HA	2.18	0.44
1:C:84[B]:ARG:HH21	1:C:139:ASN:HB3	1.83	0.43
1:C:44:ASN:O	1:C:44:ASN:ND2	2.51	0.43
1:C:115[A]:GLN:HG3	1:C:119:ASN:ND2	2.33	0.43
1:A:123:ILE:HD13	1:B:115[B]:GLN:OE1	2.18	0.43
1:C:206:LEU:O	1:C:207:THR:C	2.56	0.43
1:C:115[A]:GLN:CD	1:D:123[A]:ILE:HD13	2.39	0.43
1:B:257:ILE:HD13	1:B:257:ILE:HG21	1.82	0.43
1:C:46:GLU:CG	4:C:2026:HOH:O	2.56	0.43
1:B:99[B]:LYS:HD2	1:B:102:HIS:ND1	2.33	0.43
1:D:204:PRO:HD2	2:D:301:NAD:O2A	2.19	0.43
1:C:37:ALA:O	1:C:58:CYS:HA	2.19	0.43
1:A:200:LEU:HB2	4:A:2110:HOH:O	2.18	0.43
1:D:243:ASN:HA	1:D:244:PRO:HD3	1.90	0.43
1:C:206:LEU:CD2	3:L:350:EST:H72	2.49	0.42
1:D:112:GLU:HB3	4:D:2061:HOH:O	2.20	0.42
1:A:103:GLU:HG3	1:A:103:GLU:H	1.28	0.42
1:A:61:ALA:HA	1:A:62:PRO:HD2	1.91	0.42
1:B:187:ALA:HB3	1:B:188:PRO:HD3	2.01	0.42
1:B:16:THR:HG21	1:B:128:VAL:HG21	2.02	0.42
1:D:239:MET:CG	4:D:2109:HOH:O	2.40	0.42
1:B:187:ALA:N	1:B:188:PRO:CD	2.82	0.42
1:D:54:LEU:HA	1:D:54:LEU:HD23	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:O	1:C:109:HIS:HB2	2.19	0.42
1:C:206:LEU:HD23	3:L:350:EST:C15	2.38	0.41
1:C:12:VAL:HG23	1:C:84[A]:ARG:HH11	1.82	0.41
1:B:36[B]:THR:HG21	1:B:82:PHE:CZ	2.55	0.41
1:B:37:ALA:O	1:B:58:CYS:HA	2.22	0.40
1:B:141:PRO:HD2	4:B:2069:HOH:O	2.04	0.40
1:B:12:VAL:HG22	1:B:36[A]:THR:OG1	2.21	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASN:ND2	1:D:49:THR:OG1[1_565]	1.39	0.81
1:B:44:ASN:CG	1:D:49:THR:OG1[1_565]	1.90	0.30
4:B:2037:HOH:O	4:C:2026:HOH:O[1_564]	1.93	0.27
1:D:44:ASN:CB	4:B:2056:HOH:O[1_545]	1.94	0.26
1:B:44:ASN:ND2	1:D:49:THR:CB[1_565]	2.01	0.19
1:A:215:ASN:ND2	1:B:227:LEU:CD1[1_455]	2.03	0.17
1:A:69:LYS:CG	4:D:2065:HOH:O[1_565]	2.03	0.17
4:B:2058:HOH:O	4:C:2020:HOH:O[1_564]	2.05	0.15
1:C:103:GLU:OE2	1:D:104:LYS:CB[1_655]	2.09	0.11
1:C:104:LYS:O	1:D:106:ASN:CB[1_655]	2.17	0.03
4:A:2014:HOH:O	4:C:2042:HOH:O[1_565]	2.19	0.01

## 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	255/260 (98%)	245 (96%)	10 (4%)	0	100	100
1	B	254/260 (98%)	241 (95%)	13 (5%)	0	100	100
1	C	249/260 (96%)	237 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	255/260 (98%)	239 (94%)	12 (5%)	4 (2%)	12	2
All	All	1013/1040 (97%)	962 (95%)	47 (5%)	4 (0%)	39	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	ASP
1	D	207	THR
1	D	210	PRO
1	D	206	LEU

### 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	193/199 (97%)	186 (96%)	7 (4%)	42	19
1	B	199/199 (100%)	197 (99%)	2 (1%)	82	72
1	C	191/199 (96%)	186 (97%)	5 (3%)	54	32
1	D	192/199 (96%)	186 (97%)	6 (3%)	47	25
All	All	775/796 (97%)	755 (97%)	20 (3%)	55	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	GLU
1	A	84	ARG
1	A	103	GLU
1	A	105	LYS
1	A	132	VAL
1	A	206	LEU
1	B	216	PHE
1	B	220	GLN
1	C	7	SER

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Mol	Chain	Res	Type
1	C	44	ASN
1	C	204	PRO
1	C	239[A]	MET
1	C	239[B]	MET
1	D	48	GLU
1	D	80	GLU
1	D	104	LYS
1	D	189	ILE
1	D	214	ARG
1	D	230	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	107	GLN
1	A	143	GLN
1	B	260	GLN
1	C	44	ASN
1	C	102	HIS
1	C	106	ASN
1	D	44	ASN
1	D	215	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

5 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAD	A	301	-	38,48,48	1.88	10 (26%)	47,73,73	3.06	20 (42%)
2	NAD	B	301	-	38,48,48	1.52	7 (18%)	47,73,73	2.55	15 (31%)
2	NAD	C	301	-	38,48,48	2.02	12 (31%)	47,73,73	2.77	20 (42%)
2	NAD	D	301	-	38,48,48	1.74	6 (15%)	47,73,73	2.62	20 (42%)
3	EST	L	350	-	23,23,23	2.53	3 (13%)	36,36,36	2.82	17 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	301	-	-	0/22/62/62	0/5/5/5
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
2	NAD	C	301	-	-	0/22/62/62	0/5/5/5
2	NAD	D	301	-	-	0/22/62/62	0/5/5/5
3	EST	L	350	-	2/2/5/5	0/0/40/40	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	350	EST	O17-C17	-10.43	1.25	1.43
2	C	301	NAD	C4A-N3A	-4.24	1.29	1.35
2	D	301	NAD	C4A-N3A	-2.90	1.31	1.35
2	A	301	NAD	O4B-C4B	-2.82	1.38	1.45
2	B	301	NAD	C5A-C4A	-2.32	1.35	1.40
2	C	301	NAD	C2N-C3N	-2.24	1.35	1.39
2	C	301	NAD	PA-O2A	-2.14	1.45	1.54
2	C	301	NAD	C4N-C3N	2.03	1.42	1.39
2	A	301	NAD	C3N-C7N	2.07	1.53	1.50
2	B	301	NAD	C4N-C3N	2.17	1.43	1.39
2	A	301	NAD	O3B-C3B	2.35	1.48	1.43
2	B	301	NAD	C7N-N7N	2.38	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	C3B-C4B	2.41	1.59	1.53
2	C	301	NAD	O2B-C2B	2.49	1.48	1.43
3	L	350	EST	C10-C9	2.55	1.56	1.52
2	A	301	NAD	C6N-N1N	2.57	1.42	1.35
2	C	301	NAD	C3D-C4D	2.60	1.60	1.53
2	B	301	NAD	C2A-N1A	2.61	1.38	1.33
2	C	301	NAD	C2A-N1A	2.63	1.38	1.33
2	A	301	NAD	O2D-C2D	2.86	1.49	1.43
2	D	301	NAD	C3N-C7N	2.87	1.55	1.50
2	B	301	NAD	O3D-C3D	3.01	1.50	1.43
2	D	301	NAD	O2B-C2B	3.02	1.50	1.43
2	C	301	NAD	O4B-C1B	3.06	1.45	1.41
3	L	350	EST	C9-C8	3.07	1.57	1.54
2	C	301	NAD	C5N-C4N	3.10	1.45	1.38
2	C	301	NAD	C6N-N1N	3.12	1.43	1.35
2	A	301	NAD	C2A-N1A	3.31	1.40	1.33
2	A	301	NAD	O2B-C2B	3.80	1.52	1.43
2	D	301	NAD	C4N-C3N	3.85	1.45	1.39
2	B	301	NAD	C3N-C7N	3.90	1.56	1.50
2	A	301	NAD	C4N-C3N	3.98	1.46	1.39
2	B	301	NAD	C6N-N1N	3.99	1.46	1.35
2	C	301	NAD	C3N-C7N	4.41	1.57	1.50
2	D	301	NAD	O4D-C1D	4.55	1.47	1.41
2	D	301	NAD	O4B-C1B	4.93	1.47	1.41
2	A	301	NAD	O4B-C1B	4.98	1.47	1.41
2	C	301	NAD	O4D-C1D	5.90	1.48	1.41

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C5N-C4N-C3N	-9.14	108.84	120.33
2	C	301	NAD	N3A-C2A-N1A	-7.54	123.12	128.89
2	C	301	NAD	C5N-C4N-C3N	-6.76	111.83	120.33
2	B	301	NAD	C5N-C4N-C3N	-5.99	112.81	120.33
2	D	301	NAD	C5N-C4N-C3N	-5.89	112.93	120.33
2	A	301	NAD	C5N-C6N-N1N	-5.79	110.46	120.47
2	A	301	NAD	N3A-C2A-N1A	-5.55	124.65	128.89
2	C	301	NAD	C4N-C3N-C7N	-5.39	106.85	121.09
2	D	301	NAD	N3A-C2A-N1A	-5.30	124.83	128.89
2	C	301	NAD	O4D-C1D-N1N	-5.24	102.37	108.13
2	A	301	NAD	C1B-N9A-C4A	-5.01	119.39	126.94
2	B	301	NAD	O4D-C1D-N1N	-4.99	102.65	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C4N-C3N-C7N	-4.86	108.25	121.09
2	A	301	NAD	C2B-C1B-N9A	-4.85	106.88	114.29
2	D	301	NAD	C4N-C3N-C7N	-4.80	108.42	121.09
2	A	301	NAD	C3N-C7N-N7N	-4.76	112.61	117.82
2	D	301	NAD	C3N-C2N-N1N	-4.71	114.94	120.36
3	L	350	EST	C15-C16-C17	-4.67	101.14	105.75
2	D	301	NAD	O4D-C1D-N1N	-4.58	103.10	108.13
2	D	301	NAD	C1B-N9A-C4A	-4.46	120.22	126.94
2	D	301	NAD	C3N-C7N-N7N	-4.43	112.97	117.82
2	B	301	NAD	C4N-C3N-C7N	-4.32	109.69	121.09
2	B	301	NAD	C3N-C7N-N7N	-4.27	113.15	117.82
2	B	301	NAD	C3N-C2N-N1N	-4.15	115.58	120.36
2	D	301	NAD	C4B-O4B-C1B	-4.05	105.27	109.72
2	B	301	NAD	C5N-C6N-N1N	-3.55	114.33	120.47
2	D	301	NAD	C2B-C1B-N9A	-3.50	108.95	114.29
2	C	301	NAD	C3N-C2N-N1N	-3.27	116.60	120.36
2	A	301	NAD	O3B-C3B-C4B	-3.20	101.44	111.05
2	A	301	NAD	O4D-C1D-N1N	-3.18	104.64	108.13
3	L	350	EST	C18-C13-C17	-3.10	104.41	109.49
2	B	301	NAD	N3A-C2A-N1A	-3.09	126.53	128.89
2	C	301	NAD	C3N-C7N-N7N	-3.07	114.46	117.82
3	L	350	EST	C5-C10-C9	-3.02	117.18	121.05
2	C	301	NAD	C5N-C6N-N1N	-2.96	115.35	120.47
2	C	301	NAD	C4D-O4D-C1D	-2.91	106.53	109.72
2	A	301	NAD	C4B-O4B-C1B	-2.84	106.60	109.72
2	D	301	NAD	O4D-C4D-C5D	-2.81	99.26	109.32
2	B	301	NAD	O3D-C3D-C4D	-2.79	102.69	111.05
2	C	301	NAD	C4B-O4B-C1B	-2.76	106.68	109.72
2	A	301	NAD	C5B-C4B-C3B	-2.75	104.31	115.21
2	A	301	NAD	N6A-C6A-N1A	-2.42	114.01	119.20
2	D	301	NAD	C5N-C6N-N1N	-2.41	116.30	120.47
2	B	301	NAD	O3-PN-O5D	-2.38	96.62	102.94
2	D	301	NAD	C4D-O4D-C1D	-2.36	107.12	109.72
3	L	350	EST	C16-C15-C14	-2.33	100.44	105.12
2	B	301	NAD	C4D-O4D-C1D	-2.25	107.24	109.72
2	A	301	NAD	C3N-C2N-N1N	-2.25	117.77	120.36
2	C	301	NAD	O3D-C3D-C2D	-2.19	104.71	111.83
2	D	301	NAD	O3-PN-O5D	-2.14	97.27	102.94
2	C	301	NAD	O4B-C4B-C5B	-2.08	101.89	109.32
2	C	301	NAD	C1B-N9A-C4A	-2.03	123.87	126.94
2	A	301	NAD	O4B-C4B-C5B	-2.03	102.05	109.32
2	A	301	NAD	O2N-PN-O3	2.06	114.42	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	C4A-C5A-N7A	2.08	111.40	109.48
2	C	301	NAD	O3B-C3B-C2B	2.13	118.76	111.83
2	B	301	NAD	O2N-PN-O3	2.17	114.94	105.09
3	L	350	EST	C16-C17-C13	2.19	106.28	104.58
2	D	301	NAD	O3-PA-O5B	2.22	108.83	102.94
2	C	301	NAD	C2A-N1A-C6A	2.33	122.92	118.77
2	C	301	NAD	C2N-C3N-C7N	2.34	126.10	119.31
2	B	301	NAD	O4D-C4D-C3D	2.40	109.97	105.15
2	A	301	NAD	O7N-C7N-C3N	2.41	122.22	119.59
2	D	301	NAD	C2N-C3N-C7N	2.44	126.40	119.31
3	L	350	EST	C11-C9-C8	2.49	114.72	111.30
3	L	350	EST	C18-C13-C14	2.51	116.66	111.75
2	C	301	NAD	O3-PA-O5B	2.65	109.96	102.94
2	A	301	NAD	C2N-C3N-C7N	2.66	127.04	119.31
2	D	301	NAD	O2N-PN-O1N	2.68	127.04	112.53
3	L	350	EST	C7-C6-C5	2.70	117.94	112.86
2	A	301	NAD	C4D-O4D-C1D	2.72	112.71	109.72
2	C	301	NAD	C4A-C5A-N7A	2.74	112.00	109.48
3	L	350	EST	C7-C8-C14	2.95	116.90	112.02
3	L	350	EST	C15-C14-C13	2.96	107.67	103.82
2	D	301	NAD	O7N-C7N-N7N	3.11	126.97	122.59
3	L	350	EST	C14-C13-C17	3.35	102.86	99.28
2	C	301	NAD	C6N-C5N-C4N	3.50	124.73	119.44
2	C	301	NAD	O7N-C7N-N7N	3.82	127.97	122.59
2	D	301	NAD	C6N-C5N-C4N	3.84	125.25	119.44
3	L	350	EST	O17-C17-C16	3.95	120.49	111.56
3	L	350	EST	C9-C8-C14	4.92	116.33	108.88
3	L	350	EST	C13-C14-C8	4.98	122.16	114.37
3	L	350	EST	C11-C9-C10	4.99	119.68	113.72
2	B	301	NAD	C6N-C5N-C4N	5.06	127.09	119.44
3	L	350	EST	O17-C17-C13	5.52	126.17	114.78
2	A	301	NAD	C2N-C3N-C4N	5.76	124.70	118.29
2	B	301	NAD	O7N-C7N-C3N	6.13	126.28	119.59
2	D	301	NAD	C2N-C3N-C4N	6.17	125.17	118.29
2	B	301	NAD	C2N-C3N-C4N	6.39	125.40	118.29
3	L	350	EST	C15-C14-C8	7.04	130.15	119.03
2	C	301	NAD	C2N-C3N-C4N	7.85	127.03	118.29
2	A	301	NAD	C6N-C5N-C4N	8.11	131.69	119.44

All (2) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
3	L	350	EST	C14
3	L	350	EST	C17

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NAD	2	0
2	D	301	NAD	1	0
3	L	350	EST	11	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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