



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LDE
Title : HORSE LIVER ALCOHOL DEHYDROGENASE COMPLEXED TO NADH
AND N-FORMYL PIPERDINE
Authors : Ramaswamy, S.; Plapp, B.V.
Deposited on : 1996-12-25
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

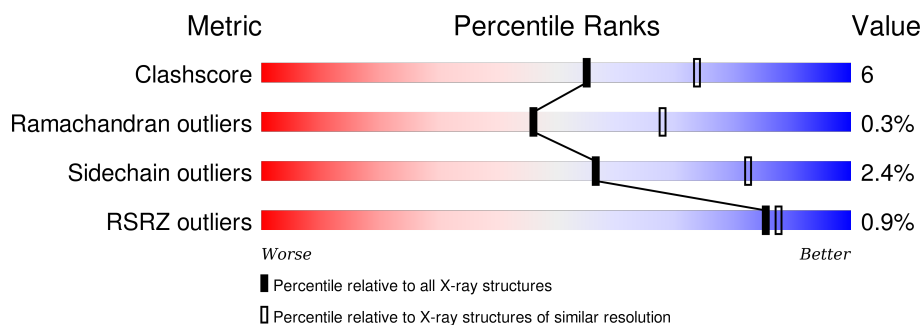
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 ≥ 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>%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> </div> </div>
1	B	374	<div> <div></div> <div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
1	C	374	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>
1	D	374	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>.</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11912 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.

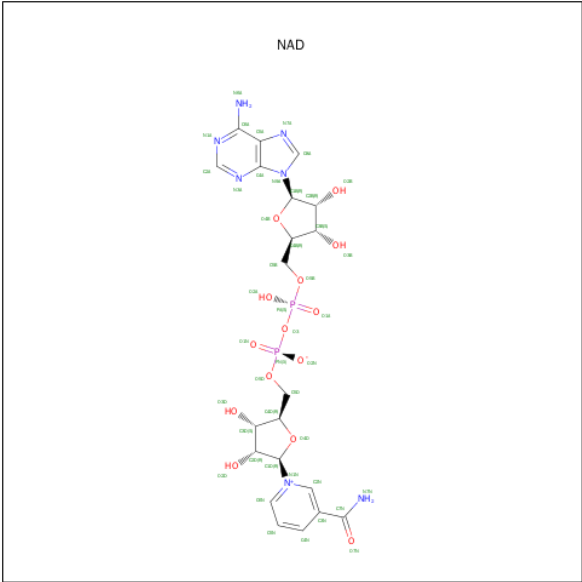
- Molecule 1 is a protein called LIVER ALCOHOL DEHYDROGENASE.

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).

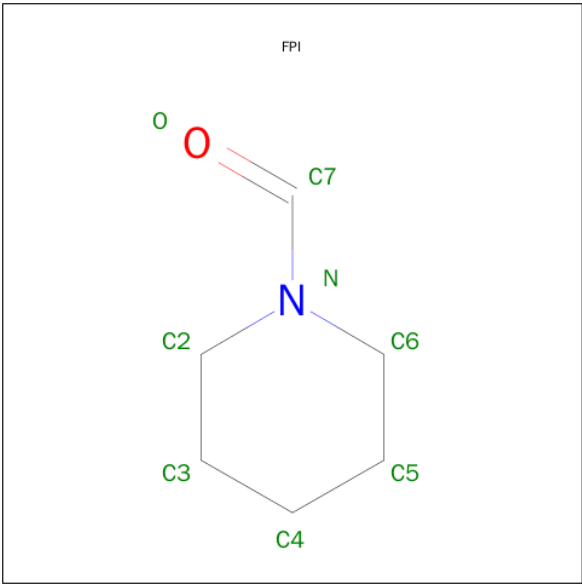
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 N-FORMYLPYPERIDINE (three-letter code: FPI) (formula: C₆H₁₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	6	1	1		
4	B	1	Total	C	N	O	0	0
			8	6	1	1		
4	C	1	Total	C	N	O	0	0
			8	6	1	1		
4	D	1	Total	C	N	O	0	0
			8	6	1	1		

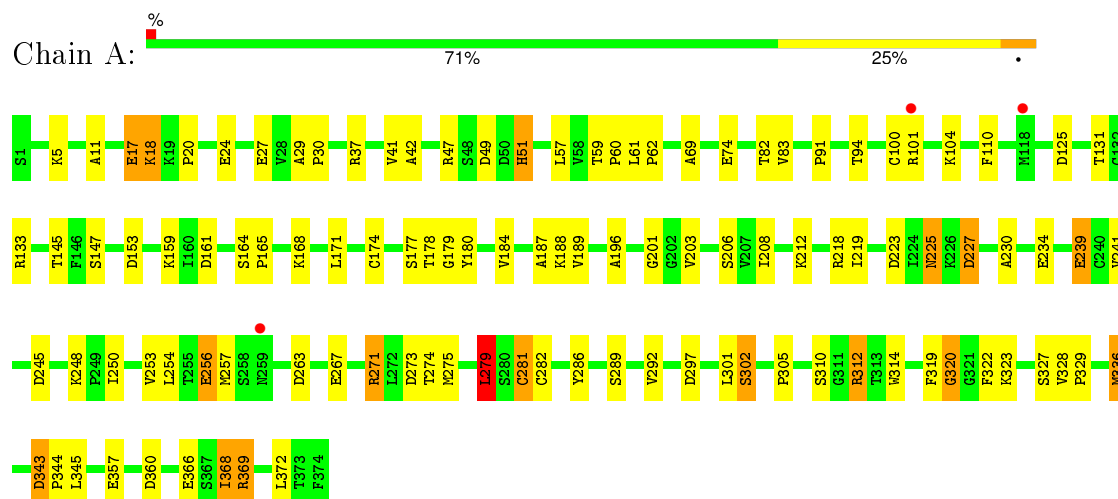
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	0
			144	144		
5	B	144	Total	O	0	0
			144	144		
5	C	134	Total	O	0	0
			134	134		
5	D	134	Total	O	0	0
			134	134		

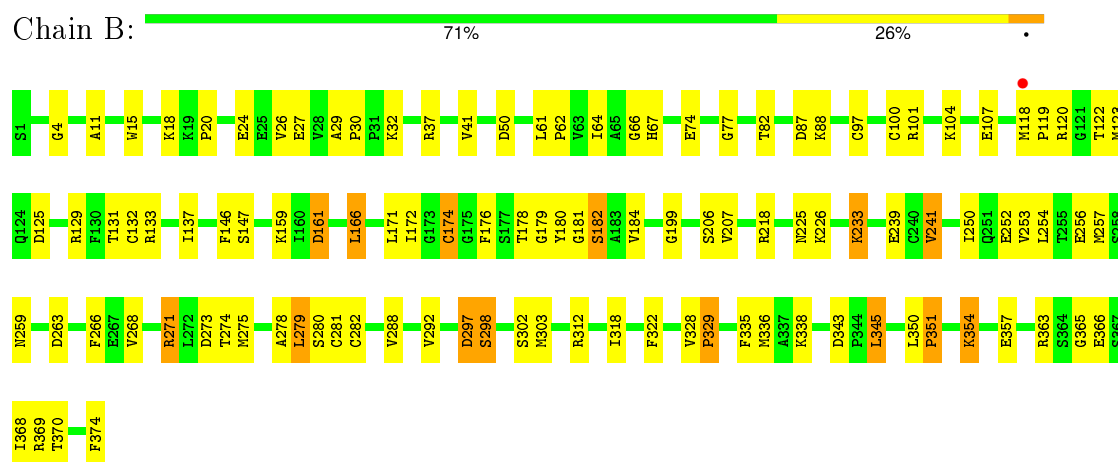
3 Residue-property plots

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.

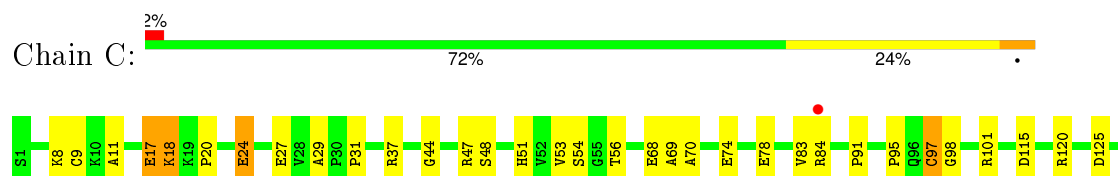
• Molecule 1: LIVER ALCOHOL DEHYDROGENASE

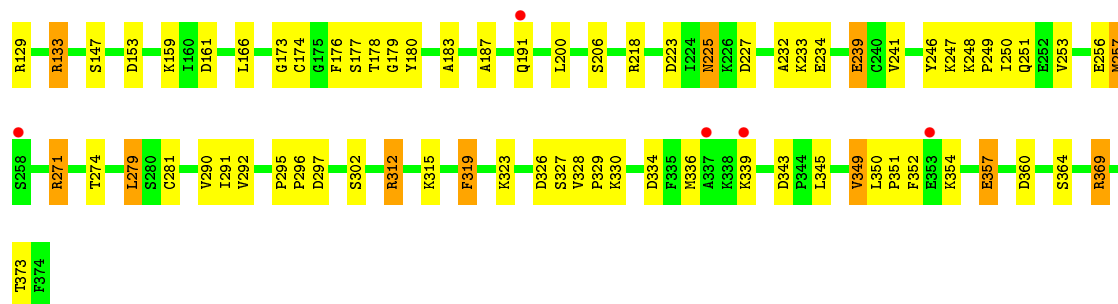


• Molecule 1: LIVER ALCOHOL DEHYDROGENASE

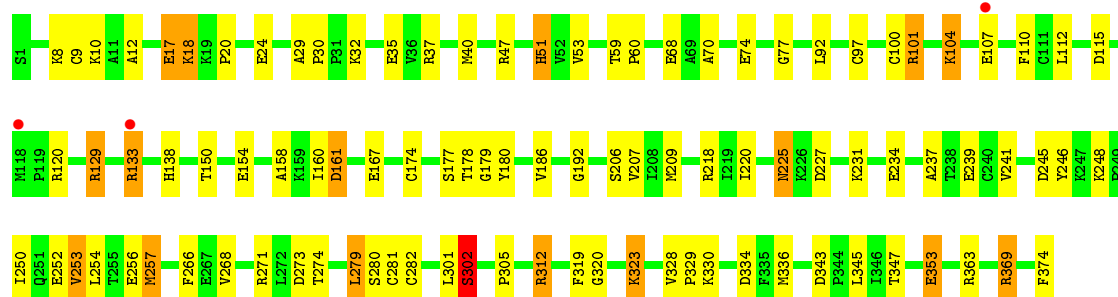
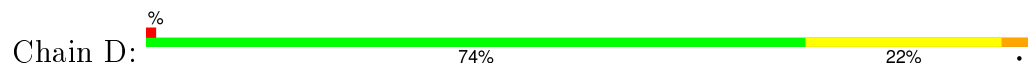


• Molecule 1: LIVER ALCOHOL DEHYDROGENASE





• 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, α , β , γ	49.93Å 180.20Å 86.80Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-2.50) 88.4 (19.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.42 (at 2.50Å)	Xtriage
Refinement program	ARP/WARP, REFMAC	Depositor
R, R_{free}	0.205 , 0.256 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.4	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 44728 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11912	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 68.07 % 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 4.6440e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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, FPI, 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	1.43	9/2837 (0.3%)	2.14	72/3834 (1.9%)
1	B	1.42	4/2837 (0.1%)	1.98	77/3834 (2.0%)
1	C	1.41	7/2837 (0.2%)	1.99	67/3834 (1.7%)
1	D	1.42	3/2837 (0.1%)	1.96	68/3834 (1.8%)
All	All	1.42	23/11348 (0.2%)	2.02	284/15336 (1.9%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	SER	CB-OG	6.72	1.50	1.42
1	C	9	CYS	CB-SG	6.67	1.93	1.82
1	C	357	GLU	CD-OE2	6.50	1.32	1.25
1	B	182	SER	CB-OG	6.49	1.50	1.42
1	C	364	SER	CA-CB	6.08	1.62	1.52
1	A	322	PHE	CG-CD2	-6.06	1.29	1.38
1	A	327	SER	CA-CB	6.06	1.62	1.52
1	A	165	PRO	N-CD	5.96	1.56	1.47
1	B	66	GLY	N-CA	-5.96	1.37	1.46
1	C	369	ARG	NE-CZ	5.93	1.40	1.33
1	A	177	SER	CA-CB	-5.91	1.44	1.52
1	B	122	THR	N-CA	-5.89	1.34	1.46
1	D	51	HIS	C-O	5.87	1.34	1.23
1	A	357	GLU	CB-CG	-5.73	1.41	1.52
1	A	286	TYR	CG-CD2	5.70	1.46	1.39
1	D	167	GLU	CD-OE2	5.33	1.31	1.25
1	C	44	GLY	C-O	5.31	1.32	1.23
1	A	51	HIS	CE1-NE2	5.29	1.44	1.32
1	A	281	CYS	CB-SG	5.17	1.91	1.82
1	C	31	PRO	N-CD	-5.11	1.40	1.47
1	C	68	GLU	CD-OE2	5.05	1.31	1.25
1	D	280	SER	CB-OG	5.05	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	SER	CA-CB	-5.02	1.45	1.52

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH2	-36.31	102.14	120.30
1	B	133	ARG	NE-CZ-NH2	22.41	131.50	120.30
1	A	133	ARG	NE-CZ-NH2	20.87	130.74	120.30
1	B	101	ARG	NE-CZ-NH1	-19.89	110.36	120.30
1	A	101	ARG	CD-NE-CZ	-18.61	97.55	123.60
1	D	133	ARG	NE-CZ-NH2	17.28	128.94	120.30
1	C	101	ARG	NE-CZ-NH1	-16.92	111.84	120.30
1	A	101	ARG	NH1-CZ-NH2	16.16	137.18	119.40
1	A	312	ARG	NE-CZ-NH1	-15.88	112.36	120.30
1	D	363	ARG	NE-CZ-NH1	-14.68	112.96	120.30
1	A	369	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	C	133	ARG	NE-CZ-NH2	14.38	127.49	120.30
1	D	101	ARG	NE-CZ-NH1	-14.11	113.25	120.30
1	D	239	GLU	OE1-CD-OE2	13.28	139.24	123.30
1	A	101	ARG	CG-CD-NE	-13.15	84.18	111.80
1	C	360	ASP	CB-CG-OD1	13.07	130.06	118.30
1	A	37	ARG	NE-CZ-NH1	-12.77	113.92	120.30
1	A	74	GLU	OE1-CD-OE2	-12.69	108.07	123.30
1	C	129	ARG	NE-CZ-NH2	12.20	126.40	120.30
1	B	218	ARG	NE-CZ-NH1	-12.15	114.23	120.30
1	C	369	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	101	ARG	NE-CZ-NH2	11.83	126.22	120.30
1	A	271	ARG	NE-CZ-NH1	11.57	126.08	120.30
1	D	47	ARG	NE-CZ-NH2	-11.29	114.66	120.30
1	D	129	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	B	369	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	C	312	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	A	125	ASP	CB-CG-OD1	10.35	127.62	118.30
1	B	125	ASP	CB-CG-OD1	10.27	127.54	118.30
1	C	47	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	C	120	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	D	115	ASP	CB-CG-OD1	9.99	127.29	118.30
1	D	343	ASP	CB-CG-OD1	9.67	127.00	118.30
1	A	125	ASP	CB-CG-OD2	-9.54	109.71	118.30
1	A	297	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	A	369	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	C	101	ARG	NH1-CZ-NH2	9.20	129.52	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	47	ARG	NE-CZ-NH2	9.00	124.80	120.30
1	A	263	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	C	334	ASP	CB-CG-OD2	8.78	126.21	118.30
1	C	115	ASP	CB-CG-OD1	8.76	126.18	118.30
1	A	312	ARG	NE-CZ-NH2	8.71	124.65	120.30
1	B	24	GLU	OE1-CD-OE2	8.70	133.74	123.30
1	A	49	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	297	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	C	37	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	A	218	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	360	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	D	369	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	24	GLU	OE1-CD-OE2	8.38	133.35	123.30
1	B	87	ASP	CB-CG-OD2	8.38	125.84	118.30
1	C	343	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	286	TYR	CB-CG-CD2	-8.36	115.98	121.00
1	B	133	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	C	84	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	256	GLU	OE1-CD-OE2	-8.07	113.61	123.30
1	B	354	LYS	CD-CE-NZ	-7.97	93.38	111.70
1	C	180	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	C	257	MET	CA-CB-CG	7.89	126.71	113.30
1	A	286	TYR	CG-CD1-CE1	-7.87	115.01	121.30
1	C	326	ASP	CB-CG-OD2	7.84	125.36	118.30
1	D	266	PHE	CB-CG-CD1	7.84	126.29	120.80
1	B	125	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	363	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	227	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	B	297	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	12	ALA	CB-CA-C	7.64	121.56	110.10
1	C	312	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	68	GLU	OE1-CD-OE2	-7.56	114.23	123.30
1	D	257	MET	CG-SD-CE	-7.54	88.13	100.20
1	C	183	ALA	CB-CA-C	-7.40	99.01	110.10
1	D	101	ARG	NH1-CZ-NH2	7.30	127.44	119.40
1	D	343	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	C	251	GLN	N-CA-CB	7.23	123.61	110.60
1	C	78	GLU	OE1-CD-OE2	7.21	131.95	123.30
1	A	153	ASP	CB-CG-OD2	7.18	124.76	118.30
1	C	271	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	360	ASP	CB-CG-OD1	7.12	124.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	172	ILE	O-C-N	-7.04	111.24	123.20
1	C	17	GLU	O-C-N	-7.01	111.48	122.70
1	A	47	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
1	C	125	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	266	PHE	CB-CG-CD1	6.86	125.60	120.80
1	B	184	VAL	O-C-N	-6.84	111.75	122.70
1	C	360	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	84	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	47	ARG	CD-NE-CZ	-6.76	114.13	123.60
1	C	234	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	A	133	ARG	NH1-CZ-NH2	-6.70	112.03	119.40
1	D	218	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	B	298	SER	N-CA-CB	-6.66	100.50	110.50
1	C	191	GLN	OE1-CD-NE2	6.66	137.21	121.90
1	B	50	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	246	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	B	239	GLU	CG-CD-OE2	-6.61	105.08	118.30
1	C	47	ARG	NH1-CZ-NH2	-6.57	112.17	119.40
1	A	336	MET	CA-CB-CG	6.55	124.44	113.30
1	D	239	GLU	CG-CD-OE1	-6.54	105.21	118.30
1	C	239	GLU	CB-CA-C	-6.53	97.35	110.40
1	B	374	PHE	CB-CG-CD2	6.51	125.36	120.80
1	A	171	LEU	O-C-N	-6.47	112.34	122.70
1	D	282	CYS	CA-CB-SG	6.47	125.65	114.00
1	B	133	ARG	NH1-CZ-NH2	-6.47	112.29	119.40
1	C	187	ALA	CB-CA-C	-6.46	100.41	110.10
1	A	184	VAL	O-C-N	-6.45	112.39	122.70
1	A	227	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	297	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	74	GLU	OE1-CD-OE2	-6.36	115.66	123.30
1	A	47	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	158	ALA	N-CA-CB	6.35	118.99	110.10
1	D	133	ARG	CD-NE-CZ	-6.34	114.72	123.60
1	D	246	TYR	CG-CD2-CE2	-6.34	116.23	121.30
1	D	253	VAL	CA-CB-CG1	6.32	120.38	110.90
1	D	133	ARG	O-C-N	-6.31	112.47	123.20
1	B	159	LYS	O-C-N	-6.31	112.61	122.70
1	D	180	TYR	CZ-CE2-CD2	-6.29	114.14	119.80
1	D	245	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	372	LEU	O-C-N	6.25	132.71	122.70
1	C	251	GLN	OE1-CD-NE2	6.24	136.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	347	THR	CA-CB-CG2	-6.22	103.70	112.40
1	A	273	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	154	GLU	OE1-CD-OE2	6.20	130.74	123.30
1	A	343	ASP	CB-CG-OD1	6.19	123.88	118.30
1	D	192	GLY	CA-C-O	-6.19	109.45	120.60
1	A	17	GLU	O-C-N	-6.17	112.83	122.70
1	B	278	ALA	CB-CA-C	6.17	119.36	110.10
1	B	288	VAL	O-C-N	6.17	132.56	122.70
1	A	180	TYR	CZ-CE2-CD2	-6.16	114.26	119.80
1	A	133	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	B	207	VAL	CG1-CB-CG2	-6.11	101.12	110.90
1	B	218	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	B	37	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	259	ASN	OD1-CG-ND2	-6.10	107.87	121.90
1	B	74	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	D	186	VAL	CG1-CB-CG2	-6.09	101.16	110.90
1	C	369	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	320	GLY	CA-C-N	6.08	128.36	116.20
1	A	273	ASP	CB-CG-OD2	6.06	123.76	118.30
1	B	107	GLU	C-N-CA	-6.05	109.59	122.30
1	A	366	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	B	252	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	C	153	ASP	CB-CG-OD1	6.04	123.73	118.30
1	C	223	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	110	PHE	CG-CD2-CE2	6.02	127.42	120.80
1	C	24	GLU	N-CA-CB	-6.01	99.77	110.60
1	D	129	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	D	266	PHE	CG-CD1-CE1	6.00	127.40	120.80
1	D	374	PHE	CA-C-O	-5.97	107.55	120.10
1	B	119	PRO	N-CA-CB	5.96	110.45	103.30
1	D	239	GLU	O-C-N	5.92	132.18	122.70
1	B	256	GLU	N-CA-CB	5.92	121.26	110.60
1	D	257	MET	CA-CB-CG	5.92	123.36	113.30
1	B	199	GLY	O-C-N	5.88	132.11	122.70
1	B	4	GLY	CA-C-O	-5.86	110.05	120.60
1	B	180	TYR	CD1-CE1-CZ	-5.86	114.53	119.80
1	C	37	ARG	NH1-CZ-NH2	5.85	125.84	119.40
1	B	24	GLU	CB-CA-C	-5.85	98.69	110.40
1	B	335	PHE	CB-CG-CD1	-5.85	116.71	120.80
1	B	351	PRO	N-CA-CB	5.85	110.32	103.30
1	B	239	GLU	CG-CD-OE1	5.83	129.96	118.30
1	D	70	ALA	N-CA-CB	5.81	118.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	TRP	O-C-N	5.80	131.97	122.70
1	A	42	ALA	CB-CA-C	-5.79	101.42	110.10
1	C	176	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	D	160	ILE	O-C-N	-5.78	113.46	122.70
1	A	212	LYS	O-C-N	-5.76	113.48	122.70
1	D	334	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	120	ARG	CA-CB-CG	5.76	126.08	113.40
1	A	273	ASP	OD1-CG-OD2	-5.76	112.36	123.30
1	B	118	MET	CA-CB-CG	5.75	123.08	113.30
1	D	353	GLU	CG-CD-OE1	5.75	129.81	118.30
1	A	110	PHE	CG-CD1-CE1	5.72	127.09	120.80
1	A	223	ASP	CA-C-O	-5.72	108.08	120.10
1	D	133	ARG	NH1-CZ-NH2	-5.71	113.11	119.40
1	C	191	GLN	CG-CD-OE1	-5.71	110.17	121.60
1	C	178	THR	CA-CB-CG2	-5.71	104.41	112.40
1	B	131	THR	CA-CB-CG2	-5.70	104.43	112.40
1	B	322	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	267	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	D	323	LYS	N-CA-C	-5.68	95.67	111.00
1	A	110	PHE	CB-CG-CD2	5.67	124.77	120.80
1	C	98	GLY	CA-C-N	5.67	129.67	117.20
1	C	326	ASP	OD1-CG-OD2	-5.67	112.53	123.30
1	D	47	ARG	CD-NE-CZ	-5.66	115.67	123.60
1	B	226	LYS	O-C-N	-5.66	113.64	122.70
1	D	273	ASP	O-C-N	-5.65	113.66	122.70
1	A	133	ARG	CD-NE-CZ	5.64	131.50	123.60
1	D	209	MET	CA-CB-CG	5.64	122.89	113.30
1	D	110	PHE	CZ-CE2-CD2	-5.61	113.36	120.10
1	D	302	SER	N-CA-CB	5.59	118.89	110.50
1	B	146	PHE	O-C-N	-5.56	113.81	122.70
1	A	239	GLU	CG-CD-OE2	-5.55	107.20	118.30
1	C	239	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	C	37	ARG	CB-CA-C	5.54	121.48	110.40
1	C	352	PHE	CB-CG-CD1	5.54	124.68	120.80
1	A	282	CYS	CA-CB-SG	5.53	123.95	114.00
1	D	220	ILE	C-N-CA	-5.53	110.69	122.30
1	B	273	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	233	LYS	CA-CB-CG	5.52	125.55	113.40
1	D	37	ARG	CB-CA-C	5.51	121.42	110.40
1	D	312	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	27	GLU	CG-CD-OE1	5.50	129.29	118.30
1	A	368	ILE	N-CA-C	-5.49	96.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	THR	N-CA-CB	5.48	120.72	110.30
1	B	67	HIS	CA-CB-CG	-5.46	104.32	113.60
1	C	133	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
1	D	9	CYS	O-C-N	5.46	131.44	122.70
1	C	8	LYS	O-C-N	5.46	131.43	122.70
1	C	349	VAL	CA-CB-CG1	-5.45	102.72	110.90
1	B	174	CYS	C-N-CA	5.45	133.74	122.30
1	B	176	PHE	CA-C-O	-5.44	108.67	120.10
1	B	20	PRO	N-CA-CB	5.44	109.83	103.30
1	D	35	GLU	OE1-CD-OE2	-5.44	116.78	123.30
1	D	161	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	297	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	94	THR	N-CA-C	-5.42	96.37	111.00
1	B	41	VAL	CA-CB-CG1	-5.42	102.78	110.90
1	D	8	LYS	O-C-N	5.41	131.35	122.70
1	B	50	ASP	OD1-CG-OD2	-5.40	113.03	123.30
1	C	129	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	C	246	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	D	20	PRO	N-CD-CG	-5.40	95.10	103.20
1	D	17	GLU	O-C-N	-5.39	114.08	122.70
1	C	373	THR	OG1-CB-CG2	-5.38	97.62	110.00
1	A	314	TRP	CG-CD1-NE1	5.38	115.48	110.10
1	A	51	HIS	N-CA-CB	5.38	120.28	110.60
1	C	319	PHE	CZ-CE2-CD2	5.36	126.53	120.10
1	C	27	GLU	OE1-CD-OE2	5.36	129.73	123.30
1	B	366	GLU	CA-C-O	-5.35	108.87	120.10
1	C	29	ALA	CB-CA-C	5.35	118.12	110.10
1	D	353	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	C	291	ILE	O-C-N	5.33	131.23	122.70
1	C	54	SER	CA-C-N	5.33	126.86	116.20
1	A	82	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	5	LYS	CB-CA-C	-5.33	99.74	110.40
1	B	303	MET	CA-CB-CG	5.29	122.29	113.30
1	A	203	VAL	CA-CB-CG2	-5.29	102.97	110.90
1	B	129	ARG	CD-NE-CZ	5.29	131.00	123.60
1	B	241	VAL	N-CA-CB	-5.29	99.87	111.50
1	A	41	VAL	CA-CB-CG1	-5.28	102.98	110.90
1	D	239	GLU	CB-CA-C	-5.28	99.84	110.40
1	D	207	VAL	CA-CB-CG2	5.27	118.80	110.90
1	A	310	SER	N-CA-CB	5.26	118.40	110.50
1	D	18	LYS	O-C-N	-5.26	114.28	122.70
1	A	279	LEU	CA-CB-CG	5.25	127.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	CYS	O-C-N	-5.24	114.29	123.20
1	D	8	LYS	CA-C-O	-5.24	109.10	120.10
1	B	123	MET	N-CA-CB	5.24	120.02	110.60
1	B	120	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	263	ASP	CB-CG-OD1	5.22	122.99	118.30
1	B	166	LEU	CB-CG-CD1	-5.20	102.15	111.00
1	B	329	PRO	N-CA-CB	5.20	109.54	103.30
1	B	120	ARG	O-C-N	-5.20	114.36	123.20
1	B	120	ARG	CA-C-N	5.20	126.59	116.20
1	B	37	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	107	GLU	C-N-CA	-5.18	111.41	122.30
1	D	138	HIS	O-C-N	5.18	131.00	122.70
1	A	189	VAL	CA-CB-CG2	-5.18	103.13	110.90
1	D	104	LYS	CB-CA-C	-5.17	100.07	110.40
1	C	74	GLU	CA-CB-CG	5.15	124.73	113.40
1	D	237	ALA	N-CA-CB	5.15	117.31	110.10
1	A	320	GLY	O-C-N	-5.15	114.45	123.20
1	A	323	LYS	N-CA-C	-5.14	97.11	111.00
1	C	180	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	A	286	TYR	CD1-CE1-CZ	5.14	124.43	119.80
1	C	323	LYS	N-CA-C	-5.13	97.14	111.00
1	A	131	THR	CA-CB-CG2	-5.13	105.22	112.40
1	D	369	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
1	C	218	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	161	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	345	LEU	CB-CA-C	-5.10	100.52	110.20
1	B	82	THR	CA-CB-CG2	-5.08	105.29	112.40
1	C	17	GLU	CA-C-O	5.08	130.76	120.10
1	A	20	PRO	O-C-N	5.07	130.82	122.70
1	C	239	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	A	196	ALA	N-CA-CB	5.05	117.18	110.10
1	B	368	ILE	N-CA-C	-5.04	97.39	111.00
1	A	27	GLU	CG-CD-OE2	-5.04	108.23	118.30
1	B	120	ARG	CD-NE-CZ	5.03	130.63	123.60
1	C	180	TYR	CD1-CG-CD2	5.01	123.41	117.90
1	C	95	PRO	N-CA-CB	5.01	109.31	103.30
1	B	271	ARG	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

There are no planarity outliers.

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	39	1
1	B	2785	0	2848	29	0
1	C	2785	0	2848	38	1
1	D	2785	0	2848	42	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	24	1	0
3	B	44	0	25	2	0
3	C	44	0	25	1	0
3	D	44	0	25	1	0
4	A	8	0	11	0	0
4	B	8	0	11	1	0
4	C	8	0	11	0	0
4	D	8	0	11	0	0
5	A	144	0	0	4	0
5	B	144	0	0	2	0
5	C	134	0	0	7	0
5	D	134	0	0	3	0
All	All	11912	0	11535	144	1

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 6.

All (144) 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:231:LYS:NZ	1:D:234:GLU:OE1	1.91	1.03
1:B:253:VAL:HG12	1:B:257:MET:HE2	1.57	0.85
1:A:253:VAL:HG12	1:A:257:MET:HE2	1.60	0.81
1:D:253:VAL:HG12	1:D:257:MET:CE	2.12	0.79
1:B:253:VAL:HG12	1:B:257:MET:CE	2.16	0.74
1:C:357:GLU:HG2	5:C:491:HOH:O	1.87	0.74
1:C:253:VAL:HG12	1:C:257:MET:HE2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG12	1:A:257:MET:CE	2.19	0.73
1:B:241:VAL:HG11	1:B:250:ILE:HD11	1.69	0.72
1:A:239:GLU:HG2	5:A:390:HOH:O	1.89	0.71
1:C:253:VAL:HG12	1:C:257:MET:CE	2.20	0.70
1:C:345:LEU:O	1:C:369:ARG:HB2	1.93	0.68
1:D:225:ASN:ND2	1:D:227:ASP:H	1.91	0.68
1:A:301:LEU:HD23	1:D:305:PRO:HG3	1.77	0.67
1:D:241:VAL:HG11	1:D:250:ILE:HD11	1.75	0.66
1:C:279:LEU:HD22	1:C:312:ARG:HD3	1.77	0.66
1:D:345:LEU:O	1:D:369:ARG:HB2	1.96	0.66
1:A:305:PRO:HG3	1:D:301:LEU:HD23	1.77	0.65
1:C:241:VAL:HG11	1:C:250:ILE:HD11	1.80	0.64
1:D:253:VAL:HG12	1:D:257:MET:HE2	1.79	0.64
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.80	0.64
1:C:330:LYS:HB3	5:C:469:HOH:O	1.98	0.63
1:A:161:ASP:OD2	1:A:336:MET:HG3	1.98	0.62
1:A:241:VAL:HG11	1:A:250:ILE:HD11	1.80	0.62
1:C:69:ALA:O	1:C:91:PRO:HD2	2.01	0.61
1:C:161:ASP:OD2	1:C:336:MET:HG3	2.01	0.60
1:C:83:VAL:HG12	1:C:159:LYS:HB2	1.84	0.60
1:D:253:VAL:HG12	1:D:257:MET:HE1	1.83	0.59
1:D:279:LEU:HD22	1:D:312:ARG:HD3	1.82	0.59
1:C:350:LEU:HB3	1:C:351:PRO:HD2	1.85	0.59
1:A:302:SER:HA	1:D:301:LEU:O	2.03	0.59
1:D:10:LYS:NZ	1:D:353:GLU:HG3	2.19	0.57
1:C:239:GLU:HG2	5:C:399:HOH:O	2.04	0.56
1:C:24:GLU:OE2	1:C:133:ARG:NH2	2.39	0.56
1:D:17:GLU:O	1:D:18:LYS:HB2	2.04	0.55
1:C:328:VAL:HB	1:C:329:PRO:HD3	1.87	0.55
1:C:17:GLU:O	1:C:18:LYS:HB2	2.06	0.55
1:D:17:GLU:HB2	1:D:53:VAL:O	2.06	0.55
1:B:241:VAL:CG1	1:B:250:ILE:HD11	2.34	0.55
1:A:225:ASN:ND2	1:A:227:ASP:H	2.05	0.55
1:C:70:ALA:HB1	1:C:166:LEU:HD22	1.89	0.55
1:C:225:ASN:ND2	1:C:227:ASP:H	2.05	0.54
1:B:271:ARG:O	1:B:275:MET:HG3	2.07	0.54
1:B:161:ASP:OD2	1:B:336:MET:HG3	2.08	0.53
1:B:179:GLY:HA3	1:B:206:SER:HB2	1.90	0.53
1:B:61:LEU:HB3	1:B:62:PRO:HA	1.90	0.53
1:B:318:ILE:HD12	4:B:378:FPI:H41	1.92	0.52
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:HB2	1:C:53:VAL:O	2.09	0.52
1:B:297:ASP:O	1:B:298:SER:HB2	2.08	0.52
1:D:161:ASP:OD2	1:D:336:MET:HG3	2.10	0.52
1:D:32:LYS:O	1:D:77:GLY:HA3	2.10	0.51
1:C:20:PRO:HA	5:C:446:HOH:O	2.10	0.51
1:C:351:PRO:HG2	1:C:354:LYS:HG3	1.93	0.50
1:B:181:GLY:O	1:B:182:SER:C	2.48	0.50
1:C:357:GLU:CB	5:C:491:HOH:O	2.60	0.50
1:A:230:ALA:O	1:A:234:GLU:HG3	2.11	0.50
1:C:248:LYS:HE2	1:C:256:GLU:OE2	2.11	0.50
1:A:254:LEU:HA	1:A:257:MET:HG2	1.93	0.49
1:D:271:ARG:HB2	1:D:274:THR:OG1	2.13	0.49
1:A:248:LYS:HE2	1:A:256:GLU:OE2	2.13	0.49
1:C:179:GLY:HA3	1:C:206:SER:HB2	1.94	0.49
1:A:17:GLU:O	1:A:18:LYS:HB2	2.13	0.48
1:B:365:GLY:HA2	5:B:398:HOH:O	2.13	0.48
1:C:56:THR:HG23	1:C:296:PRO:HA	1.96	0.48
1:C:271:ARG:HB2	1:C:274:THR:OG1	2.13	0.48
1:A:29:ALA:HB1	1:A:30:PRO:HD2	1.96	0.48
1:A:69:ALA:O	1:A:91:PRO:HD2	2.15	0.47
1:D:179:GLY:HA3	1:D:206:SER:HB2	1.95	0.47
1:B:328:VAL:HB	1:B:329:PRO:HD3	1.96	0.47
1:C:177:SER:HB2	1:C:319:PHE:CE1	2.49	0.47
1:B:100:CYS:O	1:B:104:LYS:HG2	2.14	0.47
1:D:100:CYS:O	1:D:104:LYS:HG2	2.14	0.47
1:A:241:VAL:CG1	1:A:250:ILE:HD11	2.43	0.47
1:D:40:MET:CE	1:D:150:THR:HG22	2.45	0.47
1:B:11:ALA:HA	1:B:147:SER:HA	1.97	0.46
1:D:177:SER:HB2	1:D:319:PHE:CE1	2.50	0.46
1:B:279:LEU:HD22	1:B:312:ARG:HD3	1.96	0.46
1:B:254:LEU:HA	1:B:257:MET:HG2	1.96	0.46
1:A:178:THR:HA	1:A:320:GLY:N	2.30	0.46
1:A:301:LEU:O	1:D:302:SER:HA	2.16	0.46
5:A:384:HOH:O	1:D:112:LEU:HD23	2.15	0.46
1:A:301:LEU:HD12	1:A:301:LEU:C	2.36	0.46
1:D:241:VAL:CG1	1:D:250:ILE:HD11	2.43	0.46
1:A:201:GLY:HA2	5:A:397:HOH:O	2.16	0.46
1:B:171:LEU:HD13	1:B:345:LEU:HD12	1.97	0.46
1:A:279:LEU:HD22	1:A:312:ARG:HD3	1.97	0.45
1:D:248:LYS:HE2	1:D:256:GLU:OE2	2.16	0.45
1:A:11:ALA:HA	1:A:147:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:VAL:O	3:C:377:NAD:H2N	2.17	0.45
1:A:345:LEU:O	1:A:369:ARG:HB2	2.16	0.45
1:D:254:LEU:HA	1:D:257:MET:HG2	1.98	0.45
1:A:61:LEU:HA	1:A:62:PRO:C	2.38	0.45
1:B:32:LYS:O	1:B:77:GLY:HA3	2.16	0.45
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.47	0.45
1:D:178:THR:HA	1:D:320:GLY:N	2.32	0.45
1:C:173:GLY:HA3	5:C:418:HOH:O	2.17	0.45
1:D:10:LYS:NZ	1:D:353:GLU:CG	2.80	0.44
1:D:92:LEU:CD2	1:D:328:VAL:HG21	2.48	0.44
1:B:29:ALA:HB1	1:B:30:PRO:HD2	1.99	0.44
1:A:187:ALA:O	1:A:188:LYS:HB2	2.18	0.44
1:A:69:ALA:HB3	1:A:145:THR:HG21	2.00	0.43
1:B:292:VAL:O	3:B:377:NAD:H2N	2.17	0.43
5:A:522:HOH:O	1:D:101:ARG:HD2	2.18	0.43
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.18	0.43
1:A:292:VAL:O	3:A:377:NAD:H2N	2.17	0.43
1:B:338:LYS:HD3	5:B:484:HOH:O	2.17	0.43
1:C:241:VAL:CG1	1:C:250:ILE:HD11	2.48	0.43
1:D:10:LYS:HZ2	1:D:353:GLU:HG3	1.83	0.43
1:D:330:LYS:HB3	5:D:500:HOH:O	2.19	0.43
1:D:40:MET:HE3	1:D:150:THR:HG22	2.00	0.43
1:B:64:ILE:HG13	1:B:137:ILE:HG21	2.00	0.43
1:B:354:LYS:NZ	1:B:357:GLU:OE1	2.47	0.43
1:C:48:SER:HA	1:C:51:HIS:CD2	2.53	0.42
1:A:51:HIS:HB3	1:A:57:LEU:HB2	2.01	0.42
1:D:10:LYS:HZ1	1:D:353:GLU:CG	2.32	0.42
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.20	0.42
1:C:11:ALA:HA	1:C:147:SER:HA	2.00	0.42
1:D:24:GLU:OE2	1:D:133:ARG:NH2	2.52	0.42
1:D:323:LYS:HG2	5:D:456:HOH:O	2.18	0.42
1:A:83:VAL:HG12	1:A:159:LYS:HB2	2.02	0.42
1:D:29:ALA:HB1	1:D:30:PRO:HD2	2.01	0.42
1:B:88:LYS:HD3	1:B:166:LEU:HD21	2.00	0.42
1:A:328:VAL:HB	1:A:329:PRO:HD3	2.00	0.42
1:A:208:ILE:HG23	1:A:219:ILE:HG21	2.00	0.42
1:C:225:ASN:ND2	5:C:407:HOH:O	2.52	0.42
1:C:248:LYS:HB2	1:C:249:PRO:HD2	2.02	0.42
1:D:51:HIS:CD2	3:D:377:NAD:HO2N	2.38	0.42
1:A:179:GLY:HA3	1:A:206:SER:HB2	2.00	0.41
1:C:200:LEU:HD13	1:C:232:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:CYS:O	1:A:104:LYS:HG2	2.20	0.41
1:D:59:THR:HA	1:D:60:PRO:HD3	1.91	0.41
1:C:290:VAL:HA	1:C:315:LYS:O	2.20	0.41
1:B:350:LEU:HB3	1:B:351:PRO:HD2	2.02	0.41
1:C:349:VAL:O	1:C:350:LEU:HD23	2.20	0.41
1:A:271:ARG:O	1:A:275:MET:HG3	2.20	0.41
1:C:339:LYS:HA	1:C:339:LYS:HE2	2.02	0.41
1:D:252:GLU:HG3	5:D:437:HOH:O	2.21	0.41
1:A:59:THR:HA	1:A:60:PRO:HD3	1.79	0.41
1:A:168:LYS:HE2	1:A:343:ASP:OD1	2.21	0.40
1:D:32:LYS:HD2	1:D:129:ARG:NH2	2.35	0.40
1:A:178:THR:OG1	1:A:319:PHE:HA	2.21	0.40
1:A:343:ASP:N	1:A:344:PRO:CD	2.83	0.40
1:C:295:PRO:HA	1:C:296:PRO:HD3	1.88	0.40

All (1) 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:A:245:ASP:O	1:C:247:LYS:N[1_554]	2.04	0.16

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	372/374 (100%)	351 (94%)	19 (5%)	2 (0%)	34	55
1	B	372/374 (100%)	353 (95%)	18 (5%)	1 (0%)	46	68
1	C	372/374 (100%)	351 (94%)	20 (5%)	1 (0%)	46	68
1	D	372/374 (100%)	347 (93%)	24 (6%)	1 (0%)	46	68
All	All	1488/1496 (100%)	1402 (94%)	81 (5%)	5 (0%)	46	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	C	174	CYS
1	D	174	CYS
1	B	174	CYS
1	A	368	ILE

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	308/308 (100%)	302 (98%)	6 (2%)	65	87
1	B	308/308 (100%)	299 (97%)	9 (3%)	50	77
1	C	308/308 (100%)	300 (97%)	8 (3%)	54	81
1	D	308/308 (100%)	302 (98%)	6 (2%)	65	87
All	All	1232/1232 (100%)	1203 (98%)	29 (2%)	57	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	164	SER
1	A	225	ASN
1	A	279	LEU
1	A	281	CYS
1	A	302	SER
1	B	18	LYS
1	B	97	CYS
1	B	225	ASN
1	B	233	LYS
1	B	268	VAL
1	B	279	LEU
1	B	281	CYS
1	B	282	CYS
1	B	302	SER

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Mol	Chain	Res	Type
1	C	18	LYS
1	C	97	CYS
1	C	225	ASN
1	C	233	LYS
1	C	279	LEU
1	C	281	CYS
1	C	302	SER
1	C	327	SER
1	D	97	CYS
1	D	225	ASN
1	D	268	VAL
1	D	279	LEU
1	D	281	CYS
1	D	302	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	138	HIS
1	A	225	ASN
1	A	299	GLN
1	A	300	ASN
1	B	225	ASN
1	B	259	ASN
1	B	299	GLN
1	C	124	GLN
1	C	225	ASN
1	C	299	GLN
1	C	300	ASN
1	D	124	GLN
1	D	225	ASN
1	D	299	GLN
1	D	300	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 ⓘ

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	2.52	17 (44%)	47,73,73	2.74	14 (29%)
4	FPI	A	378	2	8,8,8	1.55	2 (25%)	7,9,9	1.62	3 (42%)
3	NAD	B	377	-	38,48,48	2.34	15 (39%)	47,73,73	2.57	20 (42%)
4	FPI	B	378	2	8,8,8	1.42	1 (12%)	7,9,9	1.60	2 (28%)
3	NAD	C	377	-	38,48,48	2.20	15 (39%)	47,73,73	3.06	18 (38%)
4	FPI	C	378	2	8,8,8	1.66	1 (12%)	7,9,9	0.96	0
3	NAD	D	377	-	38,48,48	2.56	15 (39%)	47,73,73	3.19	22 (46%)
4	FPI	D	378	2	8,8,8	1.35	0	7,9,9	2.44	2 (28%)

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	FPI	A	378	2	-	0/2/10/10	0/1/1/1
3	NAD	B	377	-	-	0/22/62/62	0/5/5/5
4	FPI	B	378	2	-	0/2/10/10	0/1/1/1
3	NAD	C	377	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FPI	C	378	2	-	0/2/10/10	0/1/1/1
3	NAD	D	377	-	-	0/22/62/62	0/5/5/5
4	FPI	D	378	2	-	0/2/10/10	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	O4B-C1B	-6.42	1.33	1.41
3	D	377	NAD	C8A-N7A	-4.84	1.25	1.34
3	B	377	NAD	O4B-C1B	-4.00	1.36	1.41
3	A	377	NAD	O2B-C2B	-3.55	1.34	1.43
3	C	377	NAD	O2B-C2B	-3.50	1.34	1.43
3	B	377	NAD	O2B-C2B	-3.40	1.34	1.43
3	A	377	NAD	C2N-C3N	-3.35	1.33	1.39
3	D	377	NAD	C2A-N1A	-3.26	1.27	1.33
3	D	377	NAD	O2B-C2B	-3.17	1.35	1.43
3	D	377	NAD	PN-O2N	-3.12	1.41	1.54
3	A	377	NAD	O3D-C3D	-3.09	1.35	1.43
3	C	377	NAD	PN-O2N	-2.80	1.43	1.54
3	A	377	NAD	C2B-C3B	-2.76	1.45	1.53
3	B	377	NAD	PN-O1N	-2.64	1.41	1.51
3	C	377	NAD	O3D-C3D	-2.40	1.37	1.43
3	A	377	NAD	PA-O2A	-2.27	1.45	1.54
3	B	377	NAD	C5B-C4B	-2.23	1.44	1.51
3	C	377	NAD	C5D-C4D	-2.14	1.44	1.51
3	D	377	NAD	O2D-C2D	-2.09	1.38	1.43
3	B	377	NAD	C5D-C4D	-2.09	1.44	1.51
3	D	377	NAD	C6N-C5N	-2.08	1.34	1.38
3	B	377	NAD	C8A-N7A	-2.08	1.30	1.34
3	A	377	NAD	C5A-N7A	-2.06	1.32	1.39
3	B	377	NAD	C2N-C3N	-2.02	1.35	1.39
3	C	377	NAD	C6N-N1N	2.08	1.41	1.35
3	A	377	NAD	C6N-N1N	2.11	1.41	1.35
3	C	377	NAD	O4B-C1B	2.13	1.43	1.41
3	A	377	NAD	O4B-C4B	2.21	1.50	1.45
3	D	377	NAD	C2A-N3A	2.23	1.36	1.32
3	D	377	NAD	C4A-N3A	2.26	1.38	1.35
3	D	377	NAD	C5N-C4N	2.30	1.43	1.38
3	C	377	NAD	C2D-C3D	2.36	1.59	1.53
4	A	378	FPI	C3-C2	2.43	1.60	1.51
3	A	377	NAD	C5N-C4N	2.48	1.44	1.38
3	D	377	NAD	O4D-C1D	2.51	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	378	FPI	C4-C3	2.59	1.62	1.51
3	B	377	NAD	O4D-C4D	2.68	1.51	1.45
3	C	377	NAD	C3B-C4B	2.68	1.60	1.53
3	D	377	NAD	O4B-C4B	2.84	1.51	1.45
3	B	377	NAD	C3D-C4D	2.89	1.60	1.53
3	A	377	NAD	C3N-C7N	3.15	1.55	1.50
3	C	377	NAD	C4N-C3N	3.19	1.44	1.39
3	B	377	NAD	C6N-N1N	3.22	1.44	1.35
4	B	378	FPI	C4-C3	3.26	1.64	1.51
3	B	377	NAD	C4A-N3A	3.28	1.40	1.35
3	C	377	NAD	O4D-C4D	3.36	1.52	1.45
3	D	377	NAD	C6N-N1N	3.44	1.44	1.35
3	A	377	NAD	O4D-C1D	3.50	1.45	1.41
3	C	377	NAD	O3B-C3B	3.58	1.51	1.43
3	B	377	NAD	O4D-C1D	3.62	1.45	1.41
3	A	377	NAD	O3B-C3B	3.66	1.51	1.43
3	A	377	NAD	C4N-C3N	4.10	1.46	1.39
3	C	377	NAD	O4B-C4B	4.11	1.54	1.45
4	C	378	FPI	C2-N	4.16	1.53	1.46
3	C	377	NAD	O4D-C1D	4.18	1.46	1.41
3	A	377	NAD	C2A-N3A	4.27	1.39	1.32
3	D	377	NAD	C4N-C3N	4.33	1.46	1.39
3	A	377	NAD	C4A-N3A	4.48	1.42	1.35
3	C	377	NAD	C2A-N3A	4.68	1.40	1.32
3	C	377	NAD	C3N-C7N	4.73	1.58	1.50
3	B	377	NAD	O3B-C3B	4.79	1.54	1.43
3	A	377	NAD	O4D-C4D	4.87	1.56	1.45
3	B	377	NAD	C2A-N3A	4.93	1.40	1.32
3	B	377	NAD	C3N-C7N	5.14	1.58	1.50
3	D	377	NAD	C3N-C7N	5.93	1.59	1.50
3	D	377	NAD	O4D-C4D	7.67	1.62	1.45

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	NAD	N3A-C2A-N1A	-10.91	120.54	128.89
3	A	377	NAD	C5N-C4N-C3N	-7.73	110.62	120.33
3	D	377	NAD	N3A-C2A-N1A	-7.52	123.14	128.89
3	C	377	NAD	C3N-C2N-N1N	-6.79	112.54	120.36
3	A	377	NAD	C3N-C7N-N7N	-6.78	110.40	117.82
3	D	377	NAD	C5N-C4N-C3N	-5.87	112.95	120.33
3	C	377	NAD	C4B-O4B-C1B	-5.78	103.36	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	C4B-O4B-C1B	-5.72	103.44	109.72
3	D	377	NAD	C3N-C2N-N1N	-5.50	114.02	120.36
3	D	377	NAD	O7N-C7N-N7N	-5.42	114.97	122.59
4	D	378	FPI	C4-C5-C6	-5.25	100.87	111.26
3	B	377	NAD	C5N-C4N-C3N	-4.58	114.58	120.33
3	B	377	NAD	N3A-C2A-N1A	-4.58	125.39	128.89
3	B	377	NAD	C3N-C7N-N7N	-4.39	113.01	117.82
3	C	377	NAD	C5N-C4N-C3N	-4.17	115.09	120.33
3	D	377	NAD	O4B-C1B-N9A	-3.79	100.16	108.10
3	B	377	NAD	C3N-C2N-N1N	-3.79	116.00	120.36
3	A	377	NAD	C2B-C1B-N9A	-3.56	108.85	114.29
3	C	377	NAD	C2B-C1B-N9A	-3.41	109.08	114.29
3	A	377	NAD	C3N-C2N-N1N	-3.17	116.71	120.36
3	D	377	NAD	O4D-C1D-N1N	-3.14	104.68	108.13
3	A	377	NAD	N3A-C2A-N1A	-3.12	126.50	128.89
3	D	377	NAD	O4D-C4D-C3D	-2.81	99.49	105.15
3	D	377	NAD	C2B-C1B-N9A	-2.80	110.01	114.29
3	B	377	NAD	C5N-C6N-N1N	-2.68	115.83	120.47
3	A	377	NAD	O4D-C4D-C3D	-2.67	99.76	105.15
3	C	377	NAD	O3B-C3B-C4B	-2.65	103.11	111.05
3	B	377	NAD	O3B-C3B-C4B	-2.64	103.13	111.05
3	C	377	NAD	O7N-C7N-N7N	-2.61	118.92	122.59
3	C	377	NAD	O5D-PN-O1N	-2.57	99.66	109.62
3	D	377	NAD	C5N-C6N-N1N	-2.56	116.04	120.47
3	C	377	NAD	O4D-C4D-C5D	-2.52	100.31	109.32
3	D	377	NAD	O3-PN-O5D	-2.47	96.38	102.94
3	B	377	NAD	O3D-C3D-C4D	-2.43	103.77	111.05
3	C	377	NAD	O4B-C1B-N9A	-2.42	103.03	108.10
3	B	377	NAD	C2B-C1B-N9A	-2.40	110.62	114.29
3	D	377	NAD	C2N-C3N-C7N	-2.35	112.47	119.31
3	B	377	NAD	O4D-C4D-C3D	-2.25	100.61	105.15
3	B	377	NAD	O4B-C4B-C3B	-2.24	100.63	105.15
4	A	378	FPI	C4-C3-C2	-2.22	106.86	111.26
3	D	377	NAD	O4B-C4B-C3B	-2.21	100.69	105.15
4	A	378	FPI	C4-C5-C6	-2.13	107.05	111.26
4	B	378	FPI	C4-C5-C6	-2.12	107.06	111.26
3	D	377	NAD	O3B-C3B-C4B	-2.06	104.86	111.05
3	B	377	NAD	O3D-C3D-C2D	2.02	118.39	111.83
3	D	377	NAD	O2A-PA-O1A	2.02	123.46	112.53
3	C	377	NAD	C3N-C7N-N7N	2.02	120.03	117.82
3	B	377	NAD	C1B-N9A-C4A	2.09	130.10	126.94
3	C	377	NAD	C5D-C4D-C3D	2.11	123.57	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	N6A-C6A-N1A	2.15	123.82	119.20
4	D	378	FPI	C5-C6-N	2.18	115.13	110.54
3	A	377	NAD	O3-PN-O5D	2.36	109.19	102.94
3	B	377	NAD	C6N-C5N-C4N	2.69	123.52	119.44
4	A	378	FPI	C5-C6-N	2.74	116.32	110.54
3	D	377	NAD	C2B-C3B-C4B	2.76	108.28	102.61
3	C	377	NAD	O2A-PA-O1A	2.85	128.00	112.53
3	C	377	NAD	C2D-C3D-C4D	2.94	108.65	102.61
4	B	378	FPI	C5-C6-N	3.11	117.09	110.54
3	C	377	NAD	N6A-C6A-N1A	3.18	126.03	119.20
3	A	377	NAD	C2D-C3D-C4D	3.19	109.17	102.61
3	A	377	NAD	C2B-C3B-C4B	3.39	109.59	102.61
3	A	377	NAD	C6N-C5N-C4N	3.51	124.75	119.44
3	B	377	NAD	C2D-C3D-C4D	3.55	109.90	102.61
3	C	377	NAD	C2B-C3B-C4B	3.56	109.92	102.61
3	D	377	NAD	C6N-C5N-C4N	3.60	124.88	119.44
3	A	377	NAD	C2A-N1A-C6A	3.78	125.52	118.77
3	B	377	NAD	C2A-N1A-C6A	3.80	125.57	118.77
3	D	377	NAD	N6A-C6A-N1A	3.81	127.37	119.20
3	A	377	NAD	O2B-C2B-C3B	4.08	125.09	111.83
3	B	377	NAD	C2B-C3B-C4B	4.12	111.08	102.61
3	D	377	NAD	C2D-C3D-C4D	4.24	111.34	102.61
3	B	377	NAD	O2B-C2B-C3B	5.24	128.88	111.83
3	B	377	NAD	O7N-C7N-C3N	5.74	125.85	119.59
3	C	377	NAD	C2A-N1A-C6A	6.02	129.53	118.77
3	A	377	NAD	O7N-C7N-C3N	6.09	126.23	119.59
3	B	377	NAD	C2N-C3N-C4N	6.40	125.41	118.29
3	D	377	NAD	C2A-N1A-C6A	6.60	130.56	118.77
3	C	377	NAD	C2N-C3N-C4N	6.83	125.90	118.29
3	D	377	NAD	C3N-C7N-N7N	7.09	125.58	117.82
3	D	377	NAD	C2N-C3N-C4N	7.24	126.35	118.29
3	A	377	NAD	C2N-C3N-C4N	7.92	127.11	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NAD	1	0
3	B	377	NAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	378	FPI	1	0
3	C	377	NAD	1	0
3	D	377	NAD	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/374 (100%)	-0.30	3 (0%) 87 89	8, 16, 32, 43	0
1	B	374/374 (100%)	-0.31	1 (0%) 94 95	8, 16, 31, 42	0
1	C	374/374 (100%)	-0.17	6 (1%) 74 78	8, 16, 31, 43	0
1	D	374/374 (100%)	-0.19	3 (0%) 87 89	8, 16, 31, 43	0
All	All	1496/1496 (100%)	-0.24	13 (0%) 85 88	8, 16, 32, 43	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	MET	2.9
1	A	101	ARG	2.9
1	C	337	ALA	2.6
1	C	191	GLN	2.4
1	C	339	LYS	2.4
1	C	353	GLU	2.3
1	B	118	MET	2.2
1	C	258	SER	2.2
1	A	259	ASN	2.2
1	D	107	GLU	2.2
1	C	84	ARG	2.1
1	D	133	ARG	2.1
1	D	118	MET	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FPI	D	378	8/8	0.93	0.15	1.30	6,9,10,11	0
4	FPI	A	378	8/8	0.94	0.13	0.24	7,8,9,10	0
4	FPI	C	378	8/8	0.96	0.13	0.16	6,8,10,11	0
3	NAD	D	377	44/44	0.96	0.13	-0.12	8,13,20,21	0
4	FPI	B	378	8/8	0.97	0.11	-0.16	6,8,9,10	0
3	NAD	B	377	44/44	0.97	0.11	-0.41	7,13,21,21	0
3	NAD	C	377	44/44	0.97	0.10	-0.65	8,13,20,21	0
3	NAD	A	377	44/44	0.97	0.11	-0.83	7,14,21,22	0
2	ZN	A	376	1/1	0.98	0.03	-1.74	20,20,20,20	0
2	ZN	B	376	1/1	0.98	0.04	-2.08	19,19,19,19	0
2	ZN	C	376	1/1	0.99	0.03	-2.11	21,21,21,21	0
2	ZN	D	376	1/1	0.99	0.03	-2.14	20,20,20,20	0
2	ZN	B	375	1/1	1.00	0.02	-3.53	12,12,12,12	0
2	ZN	A	375	1/1	1.00	0.02	-3.71	12,12,12,12	0
2	ZN	D	375	1/1	1.00	0.03	-4.45	14,14,14,14	0
2	ZN	C	375	1/1	0.99	0.02	-4.83	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.