



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 11:16 PM EST

PDB ID : 9LDT
Title : DESIGN AND SYNTHESIS OF NEW ENZYMES BASED ON THE LACTATE DEHYDROGENASE FRAMEWORK
Authors : Dunn, C.R.; Holbrook, J.J.; Muirhead, H.
Deposited on : unknown
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

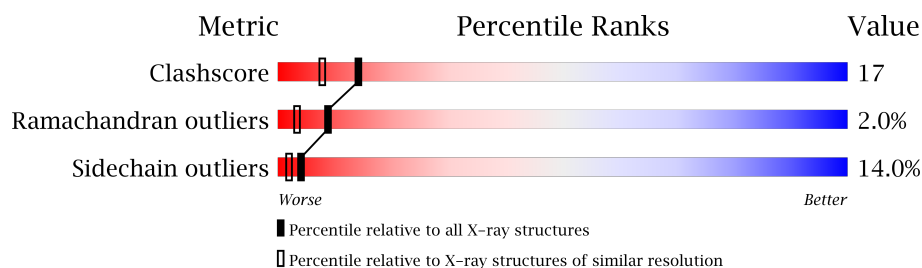
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	332	
1	B	332	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5399 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 LACTATE DEHYDROGENASE.

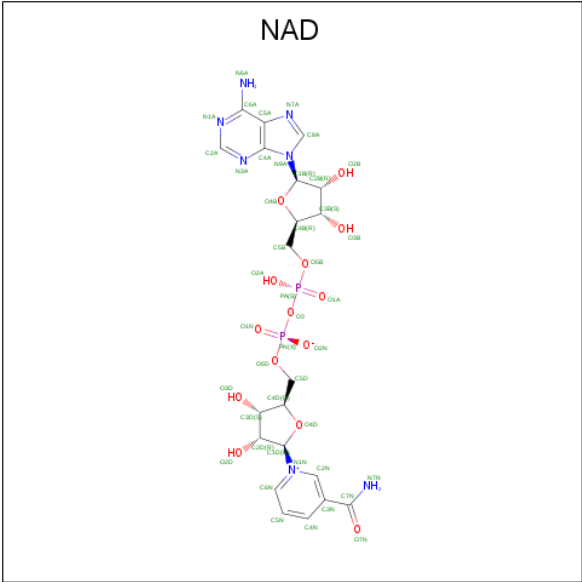
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			
1	B	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



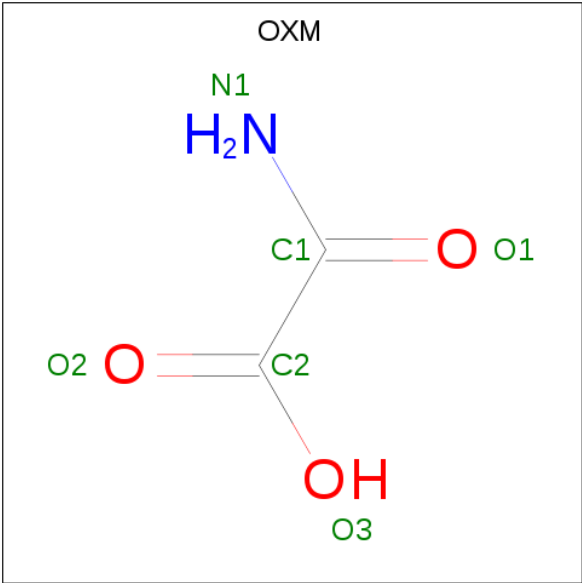
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 4 is OXAMIC ACID (three-letter code: OXM) (formula: C₂H₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	2	1	3		
4	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 5 is water.

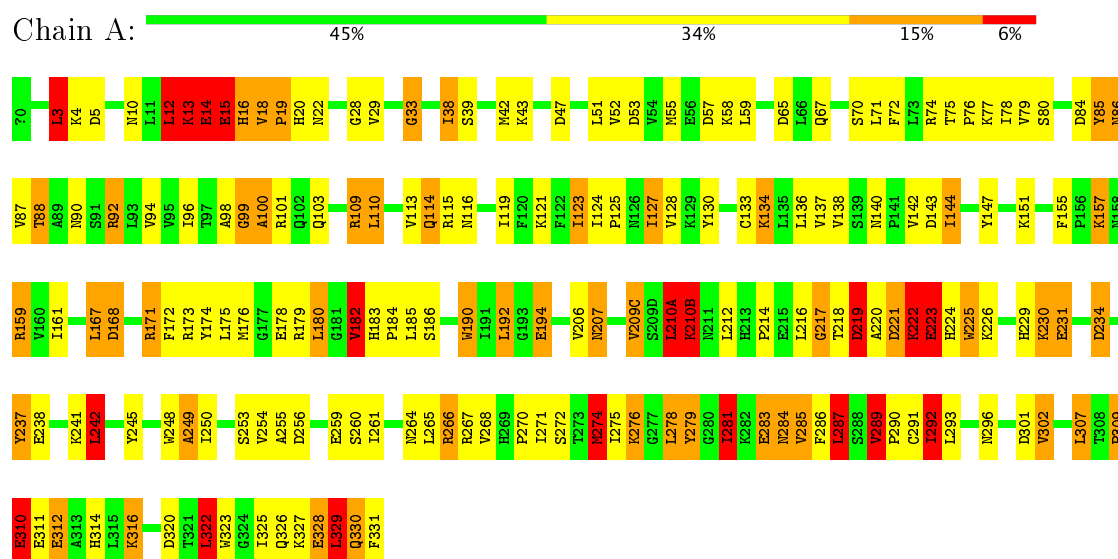
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total 76	O 76	0	0
5	B	77	Total 77	O 77	0	0

3 Residue-property plots

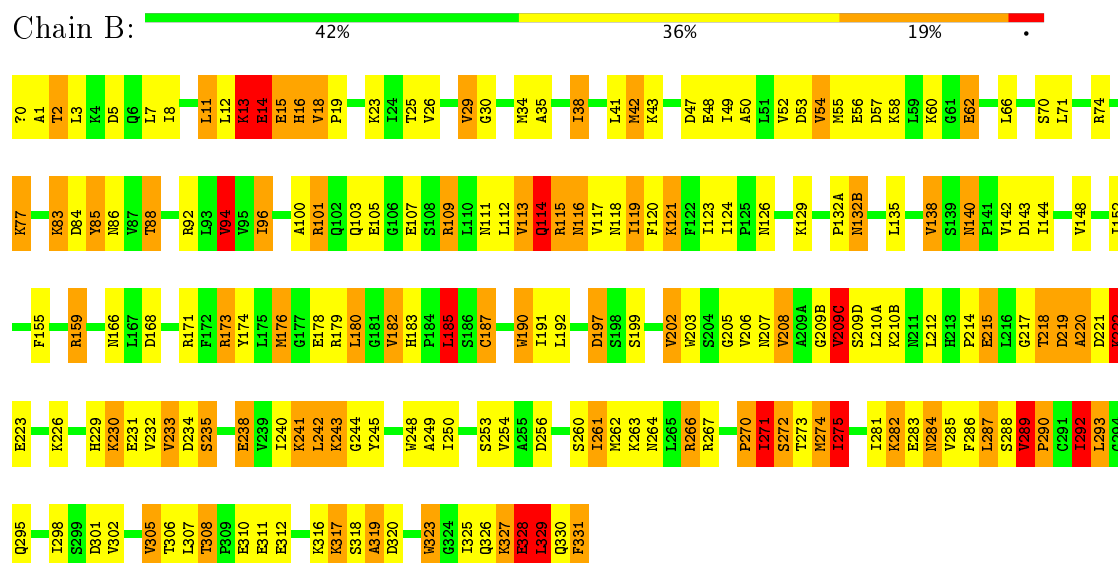
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: LACTATE DEHYDROGENASE



• Molecule 1: LACTATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.30Å 136.39Å 86.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5399	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: OXM, NAD, ACE, SO4

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	1.07	2/2615 (0.1%)	2.86	226/3541 (6.4%)
1	B	1.06	0/2615	2.88	218/3541 (6.2%)
All	All	1.06	2/5230 (0.0%)	2.87	444/7082 (6.3%)

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	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	GLU	CD-OE2	8.40	1.34	1.25
1	A	74	ARG	CZ-NH2	5.18	1.39	1.33

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH1	39.55	140.08	120.30
1	B	115	ARG	NE-CZ-NH2	39.06	139.83	120.30
1	A	159	ARG	NE-CZ-NH2	-34.14	103.23	120.30
1	A	179	ARG	NE-CZ-NH1	-28.16	106.22	120.30
1	B	221	ASP	C-N-CA	23.30	179.96	121.70
1	B	109	ARG	CD-NE-CZ	23.12	155.96	123.60
1	B	101	ARG	CD-NE-CZ	21.74	154.04	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ARG	NE-CZ-NH1	-21.32	109.64	120.30
1	B	115	ARG	NE-CZ-NH1	-18.66	110.97	120.30
1	B	11	LEU	CA-CB-CG	17.19	154.84	115.30
1	B	101	ARG	CG-CD-NE	16.04	145.47	111.80
1	B	15	GLU	CA-CB-CG	15.70	147.95	113.40
1	A	312	GLU	CA-CB-CG	15.04	146.49	113.40
1	A	179	ARG	NE-CZ-NH2	14.70	127.65	120.30
1	A	266	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	B	197	ASP	CB-CG-OD2	-13.95	105.74	118.30
1	B	219	ASP	CB-CG-OD1	13.69	130.62	118.30
1	B	292	ILE	CA-CB-CG2	13.68	138.26	110.90
1	A	256	ASP	CB-CG-OD2	-13.34	106.29	118.30
1	A	301	ASP	CB-CG-OD1	13.22	130.20	118.30
1	B	12	LEU	CA-CB-CG	13.13	145.50	115.30
1	A	221	ASP	CB-CG-OD1	13.12	130.10	118.30
1	B	317	LYS	CA-CB-CG	12.83	141.62	113.40
1	A	267	ARG	NE-CZ-NH2	-12.64	113.98	120.30
1	A	301	ASP	CB-CG-OD2	-12.47	107.07	118.30
1	A	74	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	A	312	GLU	OE1-CD-OE2	-12.28	108.56	123.30
1	B	173	ARG	NE-CZ-NH1	12.27	126.43	120.30
1	B	179	ARG	CD-NE-CZ	12.05	140.46	123.60
1	A	55	MET	CG-SD-CE	-11.60	81.64	100.20
1	B	14	GLU	CA-C-O	11.54	144.32	120.10
1	B	266	ARG	CD-NE-CZ	11.41	139.58	123.60
1	B	119	ILE	CA-CB-CG2	11.28	133.45	110.90
1	A	272	SER	N-CA-CB	10.95	126.93	110.50
1	A	16	HIS	O-C-N	10.93	140.19	122.70
1	B	301	ASP	CB-CG-OD2	-10.90	108.49	118.30
1	B	234	ASP	CB-CG-OD2	-10.84	108.54	118.30
1	A	143	ASP	CB-CG-OD1	-10.82	108.56	118.30
1	B	179	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	B	57	ASP	CB-CG-OD1	10.72	127.95	118.30
1	A	274	MET	CA-CB-CG	-10.61	95.26	113.30
1	A	42	MET	CG-SD-CE	-10.54	83.34	100.20
1	B	221	ASP	O-C-N	-10.47	105.95	122.70
1	A	168	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	A	219	ASP	CB-CG-OD1	-10.42	108.92	118.30
1	A	174	TYR	CB-CG-CD1	-10.40	114.76	121.00
1	A	267	ARG	NH1-CZ-NH2	10.38	130.82	119.40
1	A	292	ILE	CA-CB-CG2	10.29	131.48	110.90
1	A	212	LEU	CA-CB-CG	10.28	138.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ARG	NH1-CZ-NH2	10.26	130.69	119.40
1	B	105	GLU	CG-CD-OE1	10.23	138.77	118.30
1	A	173	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	267	ARG	NE-CZ-NH1	-10.21	115.19	120.30
1	B	266	ARG	NE-CZ-NH2	10.19	125.40	120.30
1	B	171	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	A	234	ASP	CB-CG-OD1	-10.05	109.26	118.30
1	B	2	THR	CA-CB-CG2	10.02	126.42	112.40
1	B	105	GLU	CG-CD-OE2	-10.00	98.31	118.30
1	A	115	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	84	ASP	CB-CG-OD1	-9.66	109.60	118.30
1	B	301	ASP	CB-CG-OD1	9.64	126.98	118.30
1	A	157	LYS	CA-CB-CG	9.44	134.16	113.40
1	A	57	ASP	CB-CG-OD1	9.42	126.78	118.30
1	B	115	ARG	NH1-CZ-NH2	-9.38	109.09	119.40
1	B	289	VAL	CB-CA-C	9.36	129.19	111.40
1	B	243	LYS	CA-C-O	-9.24	100.69	120.10
1	A	267	ARG	CD-NE-CZ	-9.21	110.70	123.60
1	B	14	GLU	CA-C-N	-9.14	97.08	117.20
1	B	208	VAL	CA-CB-CG2	9.12	124.58	110.90
1	A	86	ASN	CB-CG-OD1	-9.09	103.42	121.60
1	A	283	GLU	OE1-CD-OE2	8.93	134.02	123.30
1	A	53	ASP	CB-CG-OD2	8.93	126.33	118.30
1	B	256	ASP	CB-CG-OD1	8.91	126.32	118.30
1	A	84	ASP	CB-CG-OD2	8.85	126.26	118.30
1	A	65	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	B	57	ASP	CB-CG-OD2	-8.84	110.35	118.30
1	B	55	MET	CG-SD-CE	-8.84	86.06	100.20
1	B	101	ARG	O-C-N	-8.81	108.61	122.70
1	A	217	GLY	C-N-CA	8.73	143.53	121.70
1	B	232	VAL	CA-CB-CG1	8.71	123.97	110.90
1	B	101	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	A	245	TYR	CB-CG-CD2	8.66	126.19	121.00
1	A	172	PHE	CB-CG-CD2	8.53	126.77	120.80
1	B	260	SER	N-CA-CB	8.53	123.30	110.50
1	A	77	LYS	O-C-N	8.53	136.34	122.70
1	B	166	ASN	CB-CG-ND2	8.44	136.96	116.70
1	A	328	GLU	CA-CB-CG	8.41	131.91	113.40
1	B	292	ILE	CB-CG1-CD1	-8.35	90.52	113.90
1	A	222	LYS	CA-C-O	8.32	137.57	120.10
1	A	179	ARG	CD-NE-CZ	8.26	135.16	123.60
1	B	241	LYS	CA-CB-CG	8.26	131.57	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	CD-NE-CZ	8.21	135.10	123.60
1	A	87	VAL	CA-CB-CG2	8.14	123.10	110.90
1	B	159	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	B	16	HIS	CA-CB-CG	-8.09	99.85	113.60
1	A	13	LYS	CA-C-O	8.09	137.08	120.10
1	A	320	ASP	CA-CB-CG	8.09	131.19	113.40
1	B	289	VAL	N-CA-CB	-8.05	93.79	111.50
1	A	130	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	A	330	GLN	C-N-CA	7.98	141.64	121.70
1	B	179	ARG	NH1-CZ-NH2	-7.96	110.65	119.40
1	B	220	ALA	C-N-CA	7.94	141.54	121.70
1	B	221	ASP	CB-CG-OD1	7.94	125.44	118.30
1	B	219	ASP	CB-CA-C	7.93	126.25	110.40
1	B	85	TYR	N-CA-CB	7.90	124.82	110.60
1	B	320	ASP	CB-CG-OD1	7.89	125.40	118.30
1	B	221	ASP	N-CA-CB	-7.87	96.44	110.60
1	B	92	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	B	43	LYS	C-N-CA	7.84	141.30	121.70
1	B	209(B)	GLY	CA-C-O	-7.82	106.53	120.60
1	A	307	LEU	CA-CB-CG	7.80	133.24	115.30
1	B	176	MET	CG-SD-CE	-7.80	87.73	100.20
1	B	256	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	220	ALA	CA-C-O	-7.78	103.76	120.10
1	B	230	LYS	CD-CE-NZ	7.78	129.58	111.70
1	B	292	ILE	CB-CA-C	7.77	127.14	111.60
1	B	220	ALA	CB-CA-C	7.74	121.71	110.10
1	B	0	ACE	O-C-N	-7.66	110.45	122.70
1	B	203	TRP	N-CA-CB	7.64	124.35	110.60
1	B	48	GLU	CA-CB-CG	7.59	130.10	113.40
1	B	221	ASP	CA-CB-CG	7.51	129.91	113.40
1	B	190	TRP	O-C-N	7.47	134.66	122.70
1	A	289	VAL	N-CA-CB	-7.45	95.11	111.50
1	B	274	MET	CG-SD-CE	-7.44	88.29	100.20
1	A	143	ASP	CB-CG-OD2	7.42	124.97	118.30
1	B	92	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	92	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	329	LEU	CA-CB-CG	7.35	132.21	115.30
1	B	272	SER	N-CA-CB	7.35	121.52	110.50
1	A	86	ASN	CA-CB-CG	7.32	129.51	113.40
1	B	180	LEU	N-CA-CB	-7.32	95.76	110.40
1	A	289	VAL	CA-CB-CG1	7.31	121.87	110.90
1	B	152	ILE	CA-CB-CG1	7.31	124.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	THR	N-CA-CB	-7.25	96.52	110.30
1	A	276	LYS	CA-CB-CG	7.24	129.33	113.40
1	B	253	SER	N-CA-CB	7.21	121.31	110.50
1	B	70	SER	CA-CB-OG	-7.21	91.74	111.20
1	A	47	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	B	71	LEU	CB-CG-CD1	-7.16	98.83	111.00
1	A	77	LYS	N-CA-CB	7.15	123.47	110.60
1	B	38	ILE	CG1-CB-CG2	-7.13	95.71	111.40
1	A	223	GLU	C-N-CA	7.10	139.45	121.70
1	A	266	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	A	178	GLU	CB-CG-CD	7.09	133.34	114.20
1	A	231	GLU	OE1-CD-OE2	-7.08	114.80	123.30
1	B	272	SER	O-C-N	7.05	133.97	122.70
1	A	292	ILE	CG1-CB-CG2	-7.03	95.92	111.40
1	A	207	ASN	O-C-N	7.03	133.94	122.70
1	A	268	VAL	CA-CB-CG1	7.02	121.43	110.90
1	B	92	ARG	NH1-CZ-NH2	-7.01	111.68	119.40
1	B	205	GLY	CA-C-O	-7.01	107.98	120.60
1	B	327	LYS	O-C-N	-6.98	111.53	122.70
1	A	278	LEU	CB-CG-CD2	-6.98	99.14	111.00
1	B	119	ILE	CB-CG1-CD1	-6.97	94.38	113.90
1	A	33	GLY	CA-C-O	-6.96	108.08	120.60
1	B	86	ASN	CB-CG-ND2	6.87	133.18	116.70
1	B	287	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	A	210(A)	LEU	CA-CB-CG	6.83	131.01	115.30
1	A	289	VAL	CB-CA-C	6.79	124.30	111.40
1	A	85	TYR	CB-CG-CD1	6.74	125.04	121.00
1	A	253	SER	CA-C-N	6.74	132.02	117.20
1	A	110	LEU	CB-CG-CD2	6.73	122.44	111.00
1	B	185	LEU	CA-CB-CG	6.73	130.78	115.30
1	B	323	TRP	CB-CG-CD1	6.71	135.72	127.00
1	A	259	GLU	CG-CD-OE1	6.66	131.62	118.30
1	A	185	LEU	CA-CB-CG	6.66	130.62	115.30
1	B	307	LEU	O-C-N	6.65	133.33	122.70
1	B	243	LYS	O-C-N	6.62	134.45	123.20
1	A	237	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	223	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	A	98	ALA	N-CA-CB	-6.61	100.85	110.10
1	B	41	LEU	CB-CG-CD2	-6.60	99.77	111.00
1	A	245	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	A	171	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	A	272	SER	CB-CA-C	-6.58	97.59	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	CG-CD-OE1	6.58	131.46	118.30
1	B	221	ASP	CA-C-N	6.58	131.67	117.20
1	A	256	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	35	ALA	N-CA-CB	6.57	119.30	110.10
1	A	174	TYR	CB-CG-CD2	6.56	124.94	121.00
1	B	320	ASP	OD1-CG-OD2	-6.56	110.83	123.30
1	A	121	LYS	CA-CB-CG	6.56	127.83	113.40
1	B	5	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	84	ASP	CA-C-N	6.54	131.59	117.20
1	B	48	GLU	N-CA-CB	6.50	122.30	110.60
1	A	281	ILE	CB-CA-C	6.50	124.59	111.60
1	A	287	LEU	CB-CA-C	6.49	122.54	110.20
1	B	116	ASN	CB-CA-C	6.49	123.39	110.40
1	A	237	TYR	O-C-N	6.48	133.06	122.70
1	B	53	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	233	VAL	C-N-CA	6.47	137.88	121.70
1	A	278	LEU	CA-C-N	6.47	131.44	117.20
1	A	249	ALA	N-CA-CB	-6.45	101.07	110.10
1	B	243	LYS	N-CA-CB	6.45	122.21	110.60
1	A	328	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	A	268	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	B	14	GLU	CA-CB-CG	6.44	127.56	113.40
1	A	58	LYS	CA-CB-CG	6.44	127.56	113.40
1	B	111	ASN	CA-C-O	-6.43	106.59	120.10
1	B	222	LYS	N-CA-CB	6.43	122.17	110.60
1	A	222	LYS	N-CA-C	6.42	128.33	111.00
1	A	110	LEU	CB-CA-C	6.41	122.38	110.20
1	B	119	ILE	CG1-CB-CG2	-6.40	97.33	111.40
1	B	66	LEU	CB-CG-CD1	-6.38	100.15	111.00
1	A	155	PHE	CB-CG-CD1	-6.37	116.34	120.80
1	B	323	TRP	CD1-NE1-CE2	-6.35	103.29	109.00
1	B	266	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	134	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	B	14	GLU	C-N-CA	6.33	137.52	121.70
1	B	155	PHE	O-C-N	6.33	133.12	121.10
1	A	70	SER	CA-CB-OG	-6.33	94.12	111.20
1	A	16	HIS	CA-C-N	-6.30	103.34	117.20
1	B	319	ALA	N-CA-CB	6.30	118.92	110.10
1	A	278	LEU	CA-C-O	-6.29	106.88	120.10
1	A	13	LYS	C-N-CA	6.28	137.41	121.70
1	A	190	TRP	CD1-CG-CD2	-6.28	101.27	106.30
1	B	327	LYS	C-N-CA	6.27	137.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	O-C-N	-6.27	112.54	123.20
1	B	284	ASN	CA-CB-CG	6.26	127.18	113.40
1	B	209(C)	VAL	CA-C-O	6.26	133.24	120.10
1	A	225	TRP	O-C-N	6.25	132.70	122.70
1	B	13	LYS	CA-C-O	6.23	133.19	120.10
1	A	292	ILE	CB-CA-C	6.21	124.01	111.60
1	B	174	TYR	O-C-N	-6.20	112.78	122.70
1	B	290	PRO	CB-CA-C	6.20	127.50	112.00
1	A	302	VAL	CA-C-N	6.20	130.84	117.20
1	A	103	GLN	CB-CG-CD	6.19	127.69	111.60
1	A	231	GLU	CA-CB-CG	6.18	127.00	113.40
1	B	178	GLU	OE1-CD-OE2	6.18	130.72	123.30
1	B	26	VAL	CA-CB-CG2	6.16	120.14	110.90
1	A	238	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	B	190	TRP	NE1-CE2-CZ2	-6.16	123.63	130.40
1	A	219	ASP	OD1-CG-OD2	6.15	134.98	123.30
1	A	12	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	242	LEU	CA-C-O	-6.15	107.19	120.10
1	A	219	ASP	CA-CB-CG	6.14	126.90	113.40
1	B	111	ASN	CA-C-N	6.13	130.69	117.20
1	B	222	LYS	CB-CA-C	-6.13	98.14	110.40
1	A	222	LYS	C-N-CA	6.13	137.01	121.70
1	A	179	ARG	NH1-CZ-NH2	6.12	126.13	119.40
1	B	222	LYS	N-CA-C	6.12	127.53	111.00
1	A	79	VAL	CA-CB-CG1	6.12	120.08	110.90
1	B	112	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	B	328	GLU	CA-CB-CG	6.09	126.79	113.40
1	A	307	LEU	O-C-N	6.08	132.43	122.70
1	B	249	ALA	O-C-N	6.07	132.41	122.70
1	A	176	MET	CG-SD-CE	-6.07	90.49	100.20
1	B	13	LYS	CA-CB-CG	6.06	126.73	113.40
1	A	267	ARG	CB-CG-CD	-6.05	95.86	111.60
1	A	192	LEU	O-C-N	-6.05	112.92	123.20
1	A	67	GLN	C-N-CA	6.04	136.80	121.70
1	A	16	HIS	CB-CA-C	6.02	122.44	110.40
1	A	65	ASP	CA-C-O	-6.00	107.49	120.10
1	B	176	MET	C-N-CA	6.00	134.90	122.30
1	B	254	VAL	CA-CB-CG2	-6.00	101.91	110.90
1	A	144	ILE	CA-CB-CG1	-5.98	99.64	111.00
1	B	118	ASN	CA-CB-CG	-5.98	100.25	113.40
1	A	310	GLU	CB-CG-CD	5.97	130.32	114.20
1	B	62	GLU	OE1-CD-OE2	-5.97	116.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	O-C-N	5.97	132.25	122.70
1	B	235	SER	CB-CA-C	5.97	121.44	110.10
1	A	219	ASP	N-CA-C	5.96	127.10	111.00
1	A	100	ALA	O-C-N	5.96	132.23	122.70
1	A	190	TRP	CD1-NE1-CE2	-5.96	103.64	109.00
1	A	222	LYS	N-CA-CB	-5.95	99.88	110.60
1	A	5	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	113	VAL	CB-CA-C	5.92	122.65	111.40
1	B	318	SER	O-C-N	-5.92	113.23	122.70
1	B	329	LEU	CA-CB-CG	5.92	128.91	115.30
1	B	320	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	220	ALA	O-C-N	5.90	132.13	122.70
1	B	0	ACE	C-N-CA	5.90	136.44	121.70
1	B	312	GLU	CG-CD-OE2	-5.88	106.54	118.30
1	A	190	TRP	CB-CG-CD2	5.88	134.24	126.60
1	B	202	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	A	78	ILE	O-C-N	5.87	132.09	122.70
1	A	92	ARG	CB-CG-CD	5.87	126.86	111.60
1	B	262	MET	CG-SD-CE	-5.86	90.82	100.20
1	A	79	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	B	328	GLU	CB-CA-C	-5.85	98.69	110.40
1	B	210(A)	LEU	CB-CA-C	5.85	121.31	110.20
1	A	178	GLU	CG-CD-OE1	5.85	130.00	118.30
1	A	210(B)	LYS	CA-C-N	5.85	130.06	117.20
1	B	174	TYR	CA-CB-CG	-5.85	102.29	113.40
1	A	242	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	309	PRO	CA-C-N	5.83	130.04	117.20
1	A	101	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	A	147	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	328	GLU	CG-CD-OE1	5.80	129.90	118.30
1	A	75	THR	CA-CB-CG2	-5.80	104.28	112.40
1	A	38	ILE	CA-CB-CG2	5.79	122.48	110.90
1	B	43	LYS	CB-CG-CD	-5.78	96.56	111.60
1	A	322	LEU	CA-CB-CG	5.77	128.57	115.30
1	B	275	ILE	CA-CB-CG1	-5.74	100.10	111.00
1	A	302	VAL	O-C-N	-5.74	113.53	122.70
1	A	13	LYS	CA-CB-CG	5.73	126.01	113.40
1	A	190	TRP	CB-CG-CD1	-5.73	119.55	127.00
1	B	86	ASN	OD1-CG-ND2	-5.73	108.71	121.90
1	B	50	ALA	N-CA-CB	5.73	118.12	110.10
1	B	249	ALA	CA-C-O	-5.72	108.09	120.10
1	A	209(C)	VAL	CA-CB-CG1	5.71	119.47	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	OD1-CG-OD2	5.69	134.10	123.30
1	A	267	ARG	CG-CD-NE	-5.68	99.87	111.80
1	A	293	LEU	CA-C-N	5.68	127.56	116.20
1	B	138	VAL	CG1-CB-CG2	-5.67	101.82	110.90
1	A	261	ILE	O-C-N	-5.67	113.63	122.70
1	B	292	ILE	CA-CB-CG1	-5.67	100.23	111.00
1	A	173	ARG	NH1-CZ-NH2	5.66	125.63	119.40
1	B	241	LYS	CG-CD-CE	5.66	128.89	111.90
1	A	281	ILE	N-CA-C	-5.66	95.72	111.00
1	A	255	ALA	C-N-CA	5.65	135.82	121.70
1	A	221	ASP	CA-CB-CG	5.64	125.82	113.40
1	B	223	GLU	C-N-CA	5.62	135.75	121.70
1	B	2	THR	CA-CB-OG1	-5.61	97.21	109.00
1	B	26	VAL	O-C-N	5.61	131.68	122.70
1	A	186	SER	CA-C-O	-5.61	108.32	120.10
1	A	52	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	A	59	LEU	O-C-N	5.60	131.66	122.70
1	A	57	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	35	ALA	O-C-N	5.59	131.65	122.70
1	B	107	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	A	109	ARG	CG-CD-NE	5.58	123.52	111.80
1	B	270	PRO	CA-C-O	-5.58	106.81	120.20
1	A	283	GLU	O-C-N	5.57	131.61	122.70
1	B	182	VAL	CG1-CB-CG2	-5.55	102.02	110.90
1	B	166	ASN	OD1-CG-ND2	-5.54	109.15	121.90
1	A	267	ARG	CA-CB-CG	-5.54	101.22	113.40
1	B	261	ILE	O-C-N	-5.53	113.85	122.70
1	B	287	LEU	CA-C-O	-5.53	108.48	120.10
1	B	70	SER	CB-CA-C	-5.53	99.60	110.10
1	A	311	GLU	CG-CD-OE2	-5.52	107.25	118.30
1	B	274	MET	N-CA-CB	-5.51	100.67	110.60
1	B	114	GLN	CB-CG-CD	5.51	125.94	111.60
1	A	114	GLN	N-CA-CB	5.51	120.51	110.60
1	B	126	ASN	CB-CG-OD1	-5.51	110.59	121.60
1	A	192	LEU	N-CA-CB	-5.50	99.40	110.40
1	B	263	LYS	CA-C-O	-5.50	108.55	120.10
1	A	86	ASN	CB-CG-ND2	5.49	129.88	116.70
1	A	3	LEU	CB-CA-C	5.48	120.61	110.20
1	B	329	LEU	CB-CA-C	5.47	120.58	110.20
1	A	53	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	B	205	GLY	CA-C-N	5.46	129.22	117.20
1	A	159	ARG	CA-CB-CG	5.46	125.42	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	VAL	CA-C-N	5.45	129.19	117.20
1	B	328	GLU	CB-CG-CD	5.45	128.91	114.20
1	A	171	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	B	42	MET	CA-CB-CG	-5.45	104.04	113.30
1	A	74	ARG	CG-CD-NE	5.42	123.18	111.80
1	B	305	VAL	CB-CA-C	5.42	121.69	111.40
1	B	29	VAL	CG1-CB-CG2	-5.41	102.24	110.90
1	A	92	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	A	167	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	B	323	TRP	CB-CG-CD2	-5.40	119.58	126.60
1	A	14	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	A	137	VAL	O-C-N	5.39	131.32	122.70
1	B	74	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	B	54	VAL	CB-CA-C	-5.39	101.17	111.40
1	B	254	VAL	CG1-CB-CG2	5.38	119.51	110.90
1	A	210(B)	LYS	O-C-N	-5.38	114.09	122.70
1	B	190	TRP	CA-C-N	-5.37	105.39	117.20
1	B	94	VAL	CA-CB-CG1	5.37	118.95	110.90
1	A	109	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	250	ILE	CA-C-N	5.35	126.91	116.20
1	A	221	ASP	O-C-N	-5.35	114.14	122.70
1	A	159	ARG	CG-CD-NE	5.35	123.03	111.80
1	B	140	ASN	CB-CG-OD1	5.35	132.30	121.60
1	B	96	ILE	CA-C-N	-5.34	105.44	117.20
1	A	278	LEU	CB-CG-CD1	5.34	120.07	111.00
1	B	77	LYS	CG-CD-CE	5.33	127.88	111.90
1	B	187	CYS	N-CA-CB	5.32	120.17	110.60
1	A	285	VAL	CA-CB-CG1	5.31	118.87	110.90
1	A	207	ASN	N-CA-CB	-5.31	101.04	110.60
1	A	172	PHE	CG-CD2-CE2	5.31	126.64	120.80
1	B	271	ILE	CA-C-O	-5.30	108.96	120.10
1	B	121	LYS	CA-CB-CG	5.30	125.06	113.40
1	A	99	GLY	CA-C-N	-5.30	105.55	117.20
1	B	256	ASP	CA-C-O	5.29	131.21	120.10
1	A	18	VAL	CA-CB-CG2	-5.29	102.97	110.90
1	A	147	TYR	CA-C-O	5.29	131.20	120.10
1	A	96	ILE	CB-CG1-CD1	5.28	128.69	113.90
1	B	238	GLU	CA-C-N	5.27	128.79	117.20
1	A	260	SER	N-CA-CB	5.25	118.38	110.50
1	B	103	GLN	N-CA-C	-5.25	96.82	111.00
1	A	182	VAL	CA-CB-CG1	-5.25	103.03	110.90
1	B	323	TRP	CG-CD2-CE3	-5.24	129.18	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASN	CA-C-O	-5.24	109.10	120.10
1	A	329	LEU	C-N-CA	5.23	134.78	121.70
1	A	222	LYS	O-C-N	-5.23	114.34	122.70
1	B	209(C)	VAL	CB-CA-C	5.23	121.33	111.40
1	B	263	LYS	CD-CE-NZ	-5.22	99.70	111.70
1	A	59	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	123	ILE	O-C-N	5.21	131.03	122.70
1	A	248	TRP	CB-CG-CD2	5.20	133.36	126.60
1	B	113	VAL	CA-CB-CG1	5.20	118.70	110.90
1	A	88	THR	CA-CB-OG1	-5.20	98.08	109.00
1	B	47	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	194	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	A	264	ASN	CB-CG-OD1	5.18	131.95	121.60
1	A	279	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	259	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	B	12	LEU	CB-CA-C	-5.17	100.37	110.20
1	B	180	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	B	208	VAL	CG1-CB-CG2	-5.17	102.64	110.90
1	A	86	ASN	N-CA-CB	-5.16	101.31	110.60
1	B	144	ILE	CA-C-N	5.16	128.56	117.20
1	A	13	LYS	CA-C-N	-5.16	105.85	117.20
1	A	279	TYR	CG-CD1-CE1	5.16	125.42	121.30
1	A	72	PHE	CZ-CE2-CD2	-5.15	113.92	120.10
1	B	168	ASP	O-C-N	5.14	130.93	122.70
1	B	248	TRP	CD1-NE1-CE2	-5.14	104.37	109.00
1	A	20	HIS	O-C-N	5.14	130.92	122.70
1	B	261	ILE	CA-C-N	5.14	128.50	117.20
1	B	5	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	291	CYS	N-CA-CB	5.13	119.84	110.60
1	A	221	ASP	CA-C-O	5.13	130.87	120.10
1	B	143	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	182	VAL	CA-CB-CG2	5.12	118.58	110.90
1	A	85	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	12	LEU	O-C-N	5.11	130.88	122.70
1	B	263	LYS	CA-CB-CG	-5.10	102.17	113.40
1	A	289	VAL	CA-C-O	-5.10	109.39	120.10
1	B	290	PRO	O-C-N	-5.09	114.55	122.70
1	B	209(C)	VAL	CA-CB-CG2	5.09	118.53	110.90
1	B	238	GLU	CA-C-O	-5.08	109.44	120.10
1	A	67	GLN	O-C-N	-5.07	114.59	122.70
1	B	242	LEU	O-C-N	5.07	130.81	122.70
1	A	320	ASP	CB-CG-OD1	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LYS	C-N-CA	5.06	134.36	121.70
1	B	114	GLN	CB-CA-C	5.05	120.51	110.40
1	B	232	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	B	171	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	A	15	GLU	C-N-CA	-5.05	109.08	121.70
1	B	48	GLU	O-C-N	5.04	130.76	122.70
1	A	283	GLU	CA-C-N	-5.04	106.12	117.20
1	A	90	ASN	CA-C-O	5.03	130.67	120.10
1	B	220	ALA	O-C-N	-5.03	114.65	122.70
1	A	241	LYS	CA-CB-CG	5.03	124.46	113.40
1	B	306	THR	C-N-CA	5.03	134.27	121.70
1	B	191	ILE	N-CA-CB	5.03	122.36	110.80
1	A	16	HIS	N-CA-C	-5.02	97.44	111.00
1	A	18	VAL	CA-CB-CG1	5.02	118.43	110.90
1	B	96	ILE	CA-C-O	5.02	130.63	120.10
1	B	12	LEU	O-C-N	5.00	130.71	122.70
1	A	327	LYS	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	LEU	Mainchain
1	B	220	ALA	Mainchain
1	B	38	ILE	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	2568	0	2642	98	0
1	B	2568	0	2640	94	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	2	0
4	A	6	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	2	0	0
5	A	76	0	0	7	0
5	B	77	0	0	12	0
All	All	5399	0	5338	185	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 17.

All (185) 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:A:4:LYS:HG2	5:B:406:HOH:O	1.45	1.16
1:A:221:ASP:O	1:A:222:LYS:HB2	1.48	1.06
1:B:217:GLY:O	1:B:219:ASP:N	1.93	1.02
1:A:100:ALA:H	1:A:116:ASN:HD21	1.04	1.01
1:A:43:LYS:HE3	5:A:474:HOH:O	1.69	0.92
1:B:13:LYS:CG	1:B:14:GLU:H	1.83	0.89
1:A:18:VAL:HG23	1:A:19:PRO:HD2	1.53	0.89
1:B:100:ALA:H	1:B:116:ASN:HD21	1.20	0.89
5:A:479:HOH:O	1:B:2:THR:HG22	1.73	0.87
1:A:161:ILE:HG23	1:A:271:ILE:HD12	1.58	0.85
1:A:18:VAL:CG2	1:A:19:PRO:HD2	2.08	0.83
1:A:85:TYR:O	1:A:88:THR:HB	1.79	0.82
1:B:132(A):PRO:O	1:B:159:ARG:NH1	2.13	0.80
1:B:114:GLN:HG3	1:B:330:GLN:HE22	1.45	0.80
1:B:217:GLY:C	1:B:219:ASP:H	1.85	0.79
1:A:10:ASN:ND2	1:A:12:LEU:O	2.20	0.74
1:A:4:LYS:HE3	5:A:439:HOH:O	1.87	0.73
1:B:77:LYS:HE3	5:B:456:HOH:O	1.89	0.72
1:B:238:GLU:O	1:B:242:LEU:HD12	1.90	0.71
1:A:222:LYS:HG2	1:A:223:GLU:H	1.55	0.71
1:B:266:ARG:HB3	1:B:292:ILE:HD11	1.71	0.71
1:B:290:PRO:HG2	1:B:305:VAL:HG11	1.74	0.70
1:A:274:MET:HG3	1:A:286:PHE:CE2	2.26	0.70
1:A:14:GLU:C	1:A:15:GLU:O	2.28	0.70
1:B:114:GLN:HG3	1:B:330:GLN:NE2	2.07	0.69
1:B:58:LYS:NZ	5:B:472:HOH:O	2.18	0.69
1:A:242:LEU:HD21	1:B:60:LYS:HD3	1.76	0.68
1:A:175:LEU:HD13	1:A:231:GLU:HG3	1.76	0.68
1:B:329:LEU:HA	1:B:331:PHE:CE1	2.29	0.68
1:B:132(B):ASN:HA	1:B:159:ARG:NH1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HG13	1:A:302:VAL:HG13	1.77	0.66
1:B:13:LYS:HG3	1:B:14:GLU:H	1.61	0.66
1:A:221:ASP:O	1:A:222:LYS:CB	2.32	0.66
1:B:123:ILE:HG13	1:B:124:ILE:N	2.09	0.65
1:A:266:ARG:HB3	1:A:292:ILE:HD13	1.77	0.65
1:A:217:GLY:H	1:A:222:LYS:NZ	1.95	0.65
1:B:243:LYS:HE2	1:B:245:TYR:O	1.96	0.64
1:A:210(A):LEU:HD11	1:B:7:LEU:HD22	1.77	0.64
1:B:88:THR:CG2	5:B:453:HOH:O	2.45	0.64
1:A:230:LYS:HE3	5:A:421:HOH:O	1.97	0.64
1:B:100:ALA:N	1:B:116:ASN:HD21	1.94	0.63
1:B:261:ILE:HG13	1:B:293:LEU:HD13	1.81	0.63
1:A:222:LYS:CG	1:A:223:GLU:H	2.10	0.63
1:A:217:GLY:H	1:A:222:LYS:HZ2	1.47	0.62
1:A:100:ALA:N	1:A:116:ASN:HD21	1.87	0.62
1:B:176:MET:CE	1:B:206:VAL:HG11	2.30	0.61
1:B:275:ILE:CD1	1:B:281:ILE:HG13	2.30	0.61
1:A:210(A):LEU:HG	1:B:3:LEU:HD21	1.82	0.61
1:A:161:ILE:CG2	1:A:271:ILE:HD12	2.30	0.61
1:A:138:VAL:O	3:A:401:NAD:H2N	2.00	0.61
1:A:275:ILE:HD12	1:A:281:ILE:HG21	1.83	0.60
1:A:281:ILE:C	1:A:281:ILE:HD13	2.21	0.60
1:A:94:VAL:HG21	1:A:127:ILE:HD13	1.84	0.60
1:A:4:LYS:CG	5:B:406:HOH:O	2.24	0.60
1:B:329:LEU:HA	1:B:331:PHE:HE1	1.66	0.60
1:B:13:LYS:CD	1:B:14:GLU:H	2.15	0.59
1:B:199:SER:OG	1:B:229:HIS:HE1	1.85	0.59
1:A:190:TRP:CZ3	1:A:270:PRO:HD3	2.37	0.59
1:B:16:HIS:O	1:B:16:HIS:CG	2.55	0.59
1:A:316:LYS:HA	1:A:316:LYS:HE3	1.86	0.58
1:A:289:VAL:HG13	1:A:302:VAL:CG1	2.34	0.58
1:A:14:GLU:O	1:A:15:GLU:O	2.22	0.58
1:A:127:ILE:HD11	1:A:133:CYS:SG	2.44	0.57
1:B:117:VAL:HG22	1:B:148:VAL:HG21	1.86	0.57
1:B:274:MET:CG	1:B:286:PHE:CE2	2.87	0.57
1:B:190:TRP:HB3	1:B:192:LEU:HD13	1.86	0.57
1:A:289:VAL:CG1	1:A:302:VAL:HG13	2.35	0.56
1:A:13:LYS:O	1:A:15:GLU:N	2.39	0.55
1:B:182:VAL:HG23	1:B:187:CYS:SG	2.46	0.55
1:B:88:THR:HG22	5:B:453:HOH:O	2.07	0.55
1:B:182:VAL:CG2	1:B:187:CYS:SG	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ILE:O	1:B:288:SER:HA	2.07	0.54
1:B:275:ILE:HG12	1:B:287:LEU:HG	1.90	0.54
1:A:22:ASN:HD22	1:A:92:ARG:HH21	1.54	0.54
1:A:39:SER:HA	1:B:42:MET:CE	2.38	0.54
1:A:4:LYS:HD3	5:B:406:HOH:O	2.09	0.53
1:A:309:PRO:O	1:A:310:GLU:C	2.46	0.53
1:B:96:ILE:HD11	1:B:135:LEU:HD22	1.89	0.53
1:A:4:LYS:CD	5:B:406:HOH:O	2.53	0.53
1:B:274:MET:HG3	1:B:286:PHE:CE2	2.43	0.53
1:B:56:GLU:OE1	1:B:83:LYS:HE2	2.09	0.53
1:B:7:LEU:HG	1:B:8:ILE:HG13	1.91	0.53
1:B:16:HIS:ND1	1:B:16:HIS:O	2.41	0.53
1:B:308:THR:HG22	1:B:311:GLU:HG3	1.90	0.53
1:B:328:GLU:O	1:B:328:GLU:HG2	2.08	0.53
1:B:176:MET:HE1	1:B:206:VAL:HG11	1.91	0.52
1:B:29:VAL:HG12	1:B:62:GLU:HG3	1.91	0.52
1:B:285:VAL:HG21	1:B:319:ALA:HB1	1.91	0.52
1:B:120:PHE:HA	1:B:123:ILE:HG12	1.92	0.52
1:B:18:VAL:HG23	1:B:19:PRO:HD2	1.92	0.52
1:B:115:ARG:HD3	5:B:420:HOH:O	2.10	0.52
1:A:210(B):LYS:NZ	1:A:214:PRO:O	2.42	0.52
1:A:194:GLU:HG3	1:A:322:LEU:CD1	2.40	0.51
1:A:292:ILE:HD12	1:A:292:ILE:C	2.29	0.51
1:A:222:LYS:HD2	1:A:225:TRP:H	1.75	0.51
1:A:39:SER:HA	1:B:42:MET:HE3	1.90	0.51
1:B:183:HIS:ND1	1:B:185:LEU:HB2	2.26	0.51
1:A:180:LEU:HB3	1:A:182:VAL:HG23	1.93	0.51
1:A:287:LEU:C	1:A:287:LEU:HD12	2.31	0.51
1:B:192:LEU:HD22	1:B:202:VAL:HG21	1.93	0.51
1:B:215:GLU:O	1:B:219:ASP:HB2	2.11	0.51
1:B:77:LYS:CE	5:B:456:HOH:O	2.52	0.50
1:A:15:GLU:O	1:A:16:HIS:CD2	2.65	0.49
1:A:85:TYR:CE2	1:A:127:ILE:HG22	2.48	0.49
1:A:316:LYS:HA	1:A:316:LYS:CE	2.43	0.49
1:A:51:LEU:O	1:A:80:SER:HA	2.11	0.49
1:B:29:VAL:CG1	1:B:62:GLU:HG3	2.43	0.49
1:A:127:ILE:HG13	1:A:128:VAL:N	2.27	0.49
1:B:215:GLU:HG2	1:B:222:LYS:HZ2	1.78	0.49
1:A:22:ASN:ND2	1:A:92:ARG:HH21	2.11	0.49
1:B:231:GLU:O	1:B:235:SER:HB3	2.12	0.49
1:B:328:GLU:O	1:B:330:GLN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:HB	1:A:125:PRO:HD3	1.96	0.48
1:A:99:GLY:HA2	1:A:119:ILE:HD13	1.95	0.48
1:B:266:ARG:HB3	1:B:292:ILE:CD1	2.39	0.48
1:B:275:ILE:H	1:B:275:ILE:HG13	1.56	0.47
1:A:144:ILE:HD13	1:A:325:ILE:HG21	1.95	0.47
1:A:71:LEU:HD12	1:B:185:LEU:HD13	1.96	0.47
1:A:167:LEU:HD11	1:A:249:ALA:HB1	1.96	0.47
1:A:159:ARG:HH21	1:A:159:ARG:CG	2.21	0.47
1:A:123:ILE:O	1:A:127:ILE:HG23	2.15	0.47
1:B:285:VAL:HG12	1:B:326:GLN:NE2	2.30	0.47
1:B:274:MET:HG2	1:B:286:PHE:CE2	2.49	0.47
1:A:14:GLU:O	1:A:16:HIS:HD2	1.96	0.46
1:A:217:GLY:O	1:A:219:ASP:OD2	2.33	0.46
1:A:159:ARG:HH21	1:A:159:ARG:HG3	1.81	0.46
1:A:194:GLU:HG3	1:A:322:LEU:HD13	1.97	0.46
1:A:206:VAL:HG12	1:A:210(A):LEU:HD22	1.97	0.46
1:B:109:ARG:HD3	1:B:140:ASN:OD1	2.16	0.46
1:A:28:GLY:O	1:A:33:GLY:HA3	2.16	0.46
1:A:210(A):LEU:CD1	1:B:7:LEU:HD22	2.44	0.46
1:A:279:TYR:H	1:A:281:ILE:HG22	1.81	0.46
1:A:289:VAL:CG1	1:A:302:VAL:CG1	2.94	0.46
1:B:289:VAL:HA	1:B:290:PRO:HD3	1.71	0.46
1:B:183:HIS:CE1	1:B:185:LEU:HD22	2.51	0.46
1:A:285:VAL:HG22	1:A:323:TRP:HB2	1.98	0.45
1:B:173:ARG:NE	1:B:187:CYS:O	2.49	0.45
1:A:217:GLY:N	1:A:222:LYS:NZ	2.62	0.45
1:A:171:ARG:NH2	5:A:407:HOH:O	2.49	0.45
1:A:326:GLN:HA	1:A:329:LEU:HD22	1.99	0.44
1:B:273:THR:HB	1:B:298:ILE:HD12	2.00	0.44
1:B:19:PRO:HB2	1:B:23:LYS:HB2	2.00	0.44
1:B:240:ILE:O	1:B:244:GLY:N	2.49	0.44
1:B:243:LYS:HE3	1:B:245:TYR:CE2	2.52	0.44
1:B:308:THR:HG23	1:B:310:GLU:OE1	2.18	0.44
1:A:283:GLU:HB3	1:A:284:ASN:H	1.60	0.44
1:B:113:VAL:O	1:B:117:VAL:HG23	2.18	0.44
1:A:276:LYS:HB2	1:A:283:GLU:O	2.18	0.44
1:A:307:LEU:HD13	1:A:312:GLU:HA	1.99	0.44
1:B:208:VAL:O	1:B:209(C):VAL:HG13	2.17	0.44
1:B:25:THR:HB	1:B:94:VAL:HB	2.00	0.44
1:A:234:ASP:HA	1:A:237:TYR:HD1	1.83	0.43
1:A:222:LYS:HB3	1:A:224:HIS:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:O	1:A:254:VAL:HG23	2.19	0.43
1:A:19:PRO:O	1:A:19:PRO:HG2	2.17	0.43
1:A:279:TYR:N	1:A:281:ILE:HG22	2.33	0.43
1:A:109:ARG:HG3	5:A:408:HOH:O	2.17	0.43
1:B:190:TRP:HE3	1:B:270:PRO:HB3	1.82	0.43
1:A:216:LEU:HA	1:A:222:LYS:HD3	2.00	0.43
1:A:190:TRP:HB3	1:A:192:LEU:HD13	2.01	0.43
1:B:115:ARG:CD	5:B:420:HOH:O	2.65	0.43
1:B:210(B):LYS:NZ	1:B:214:PRO:O	2.52	0.43
1:A:289:VAL:HA	1:A:290:PRO:HD3	1.94	0.42
1:B:140:ASN:HA	1:B:142:VAL:N	2.34	0.42
1:B:30:GLY:HA3	3:B:401:NAD:O5B	2.19	0.42
1:A:140:ASN:HA	1:A:142:VAL:N	2.34	0.42
1:B:85:TYR:O	1:B:88:THR:HB	2.20	0.42
1:A:229:HIS:HD2	5:A:419:HOH:O	2.03	0.42
1:A:13:LYS:CB	1:A:14:GLU:HG3	2.49	0.42
1:B:16:HIS:CD2	1:B:16:HIS:C	2.87	0.42
1:A:316:LYS:CA	1:A:316:LYS:CE	2.98	0.41
1:A:13:LYS:HB2	1:A:14:GLU:HG3	2.02	0.41
1:B:264:ASN:HB2	1:B:295:GLN:HB3	2.02	0.41
1:B:215:GLU:HG2	1:B:222:LYS:NZ	2.36	0.41
1:A:183:HIS:CG	1:A:184:PRO:HD2	2.56	0.41
1:B:275:ILE:HD12	1:B:281:ILE:HG21	2.02	0.41
1:B:197:ASP:HA	1:B:233:VAL:HG13	2.03	0.41
1:B:29:VAL:HG13	1:B:34:MET:SD	2.61	0.41
1:B:88:THR:HG23	5:B:453:HOH:O	2.16	0.41
1:A:110:LEU:HD22	1:A:325:ILE:HD13	2.03	0.41
1:A:38:ILE:HA	1:A:38:ILE:HD12	1.88	0.41
1:B:138:VAL:O	3:B:401:NAD:H2N	2.21	0.40
1:B:282:LYS:HD2	1:B:283:GLU:OE1	2.21	0.40
1:A:14:GLU:O	1:A:16:HIS:CD2	2.74	0.40
1:A:3:LEU:C	1:A:3:LEU:HD12	2.41	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:B:132(B):ASN:OD1	1:B:132(B):ASN:OD1[2_655]	1.53	0.67

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	330/332 (99%)	301 (91%)	23 (7%)	6 (2%)	10	4
1	B	330/332 (99%)	304 (92%)	19 (6%)	7 (2%)	8	3
All	All	660/664 (99%)	605 (92%)	42 (6%)	13 (2%)	9	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	218	THR
1	A	222	LYS
1	A	330	GLN
1	B	1	ALA
1	B	14	GLU
1	B	218	THR
1	B	222	LYS
1	B	329	LEU
1	A	15	GLU
1	B	15	GLU
1	A	219	ASP
1	B	284	ASN

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	285/285 (100%)	246 (86%)	39 (14%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	285/285 (100%)	244 (86%)	41 (14%)	4	2
All	All	570/570 (100%)	490 (86%)	80 (14%)	4	2

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	LEU
1	A	13	LYS
1	A	14	GLU
1	A	15	GLU
1	A	19	PRO
1	A	76	PRO
1	A	86	ASN
1	A	114	GLN
1	A	127	ILE
1	A	134	LYS
1	A	136	LEU
1	A	151	LYS
1	A	157	LYS
1	A	168	ASP
1	A	180	LEU
1	A	182	VAL
1	A	207	ASN
1	A	209(C)	VAL
1	A	210(A)	LEU
1	A	210(B)	LYS
1	A	223	GLU
1	A	226	LYS
1	A	230	LYS
1	A	242	LEU
1	A	274	MET
1	A	278	LEU
1	A	281	ILE
1	A	284	ASN
1	A	287	LEU
1	A	289	VAL
1	A	292	ILE
1	A	310	GLU
1	A	314	HIS
1	A	316	LYS
1	A	322	LEU

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Mol	Chain	Res	Type
1	A	328	GLU
1	A	329	LEU
1	A	331	PHE
1	B	11	LEU
1	B	13	LYS
1	B	18	VAL
1	B	49	ILE
1	B	52	VAL
1	B	54	VAL
1	B	83	LYS
1	B	94	VAL
1	B	101	ARG
1	B	114	GLN
1	B	119	ILE
1	B	121	LYS
1	B	129	LYS
1	B	132(B)	ASN
1	B	180	LEU
1	B	185	LEU
1	B	207	ASN
1	B	209(C)	VAL
1	B	209(D)	SER
1	B	212	LEU
1	B	215	GLU
1	B	218	THR
1	B	226	LYS
1	B	230	LYS
1	B	241	LYS
1	B	271	ILE
1	B	272	SER
1	B	275	ILE
1	B	282	LYS
1	B	289	VAL
1	B	292	ILE
1	B	293	LEU
1	B	308	THR
1	B	316	LYS
1	B	317	LYS
1	B	323	TRP
1	B	325	ILE
1	B	327	LYS
1	B	328	GLU

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Mol	Chain	Res	Type
1	B	329	LEU
1	B	331	PHE

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	16	HIS
1	A	22	ASN
1	A	102	GLN
1	A	116	ASN
1	A	229	HIS
1	A	284	ASN
1	B	114	GLN
1	B	116	ASN
1	B	207	ASN
1	B	229	HIS
1	B	326	GLN

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 ⓘ

6 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
3	NAD	A	401	-	41,48,48	2.74	5 (12%)	43,73,73	4.76	22 (51%)
4	OXM	A	402	-	2,5,5	12.53	2 (100%)	2,6,6	13.78	2 (100%)
2	SO4	A	403	-	4,4,4	0.92	0	6,6,6	1.22	1 (16%)
3	NAD	B	401	-	41,48,48	1.88	5 (12%)	43,73,73	2.56	16 (37%)
4	OXM	B	402	-	2,5,5	11.32	2 (100%)	2,6,6	8.31	1 (50%)
2	SO4	B	403	-	4,4,4	0.93	0	6,6,6	1.05	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	401	-	-	0/22/62/62	0/5/5/5
4	OXM	A	402	-	-	0/0/4/4	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	NAD	B	401	-	-	0/22/62/62	0/5/5/5
4	OXM	B	402	-	-	0/0/4/4	0/0/0/0
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	O7N-C7N	-7.76	1.08	1.24
3	B	401	NAD	C5N-C4N	-3.97	1.31	1.38
3	A	401	NAD	C5N-C4N	-3.60	1.32	1.38
3	A	401	NAD	C2B-C1B	-3.14	1.48	1.53
3	A	401	NAD	C2N-C3N	-2.66	1.34	1.39
3	B	401	NAD	C7N-N7N	-2.45	1.28	1.33
3	B	401	NAD	C6N-N1N	3.29	1.43	1.35
3	B	401	NAD	C3N-C7N	5.02	1.58	1.50
4	B	402	OXM	O1-C1	6.09	1.36	1.24
3	A	401	NAD	C6N-N1N	6.70	1.52	1.35
4	A	402	OXM	O1-C1	7.71	1.40	1.24
3	A	401	NAD	C3N-C7N	14.02	1.72	1.50
4	B	402	OXM	C1-N1	14.81	1.61	1.33
4	A	402	OXM	C1-N1	15.95	1.64	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	OXM	O1-C1-N1	-18.36	96.46	122.58
3	A	401	NAD	O7N-C7N-C3N	-12.17	105.40	119.62
4	B	402	OXM	C2-C1-N1	-11.62	96.26	115.85
3	A	401	NAD	C3N-C7N-N7N	-8.27	108.33	117.77
3	A	401	NAD	N6A-C6A-N1A	-8.07	102.76	118.77
3	A	401	NAD	C3N-C2N-N1N	-7.14	113.24	120.43
4	A	402	OXM	C2-C1-N1	-6.51	104.87	115.85
3	A	401	NAD	C5N-C6N-N1N	-5.89	111.34	120.40
3	B	401	NAD	C3N-C7N-N7N	-5.60	111.39	117.77
3	A	401	NAD	C4B-O4B-C1B	-5.51	103.91	109.77
3	B	401	NAD	C5N-C4N-C3N	-4.46	115.11	120.35
3	A	401	NAD	C1B-N9A-C4A	-4.22	119.34	126.64
3	B	401	NAD	C4B-O4B-C1B	-4.06	105.44	109.77
3	B	401	NAD	O7N-C7N-C3N	-4.04	114.90	119.62
3	A	401	NAD	C4A-C5A-N7A	-3.84	105.70	109.41
3	A	401	NAD	N3A-C2A-N1A	-3.39	125.91	128.86
3	B	401	NAD	C2B-C3B-C4B	-3.28	96.23	102.62
3	A	401	NAD	C4N-C3N-C7N	-3.15	112.69	121.07
3	B	401	NAD	C4N-C3N-C7N	-3.12	112.77	121.07
3	B	401	NAD	O3D-C3D-C4D	-2.65	103.35	111.09
3	B	401	NAD	O4D-C4D-C5D	-2.37	101.40	109.40
3	B	401	NAD	C1B-N9A-C4A	-2.31	122.64	126.64
3	A	401	NAD	C5N-C4N-C3N	-2.30	117.64	120.35
3	A	401	NAD	C5B-C4B-C3B	-2.29	106.55	115.29
3	A	401	NAD	C4D-O4D-C1D	-2.05	107.58	109.77
2	A	403	SO4	O3-S-O1	2.25	121.64	109.26
3	A	401	NAD	O2N-PN-O5D	2.34	119.19	108.14
3	A	401	NAD	O2B-C2B-C3B	2.68	120.41	111.83
3	B	401	NAD	O5D-PN-O1N	2.83	120.66	109.25
3	A	401	NAD	O5D-PN-O1N	2.85	120.75	109.25
3	B	401	NAD	O2B-C2B-C3B	3.00	121.43	111.83
3	A	401	NAD	C6N-C5N-C4N	3.15	124.20	119.44
3	A	401	NAD	O2B-C2B-C1B	3.24	121.76	111.61
3	B	401	NAD	O2A-PA-O1A	3.31	129.40	112.28
3	B	401	NAD	O4B-C4B-C3B	3.42	111.96	105.17
3	B	401	NAD	C5A-C6A-N6A	3.45	127.51	120.47
3	A	401	NAD	O2D-C2D-C3D	3.70	123.68	111.83
3	B	401	NAD	C2N-C3N-C4N	4.82	123.76	118.26
3	B	401	NAD	O7N-C7N-N7N	7.04	132.59	122.58
3	A	401	NAD	C2N-C3N-C4N	8.47	127.93	118.26
3	A	401	NAD	C5A-C6A-N6A	9.19	139.20	120.47
3	A	401	NAD	O7N-C7N-N7N	16.64	146.25	122.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAD	1	0
3	B	401	NAD	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.