Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:40 PM EDT

PDB ID	:	9LDB
Title	:	DESIGN AND SYNTHESIS OF NEW ENZYMES BASED ON THE LACTATE DEHYDROGENASE FRAMEWORK
Authors	:	Dunn, C.R.; Holbrook, J.J.; Muirhead, H.
Deposited on	:	1991-11-26
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

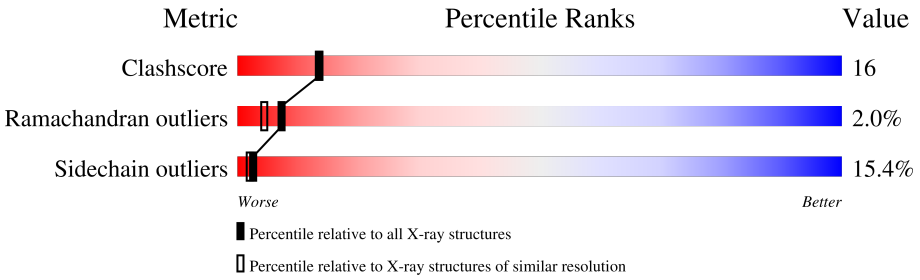
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	332	48% 32% 15% .
1	B	332	48% 33% 15% .

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
2	SO4	A	402	-	X	-	-
4	OXM	B	402	-	X	-	-

2 Entry composition

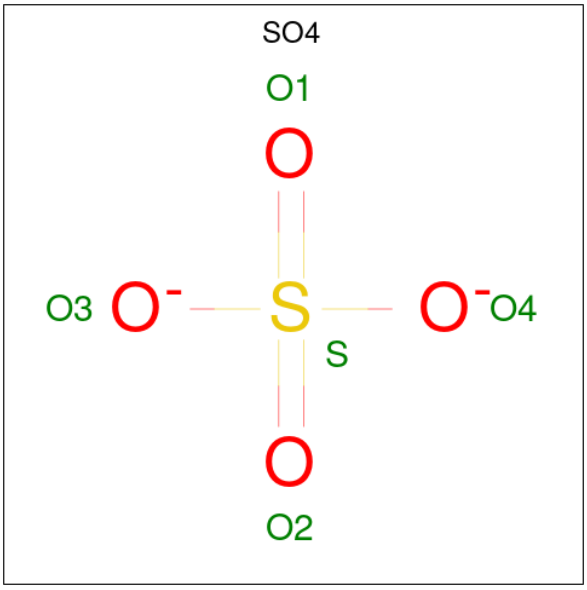
There are 5 unique types of molecules in this entry. The entry contains 5396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

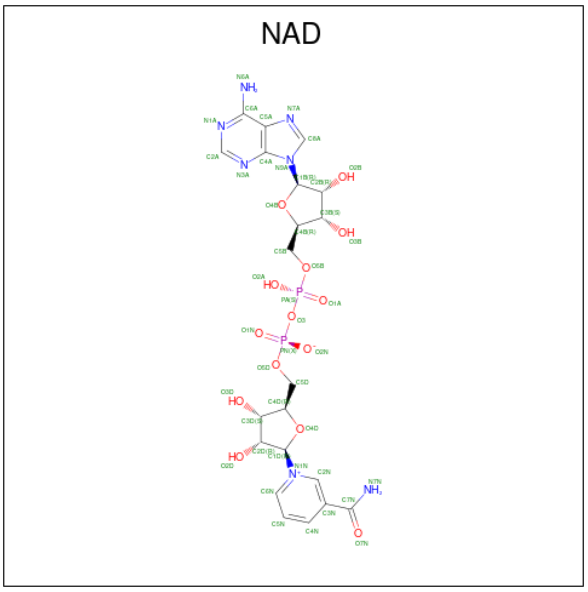
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			
1	B	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



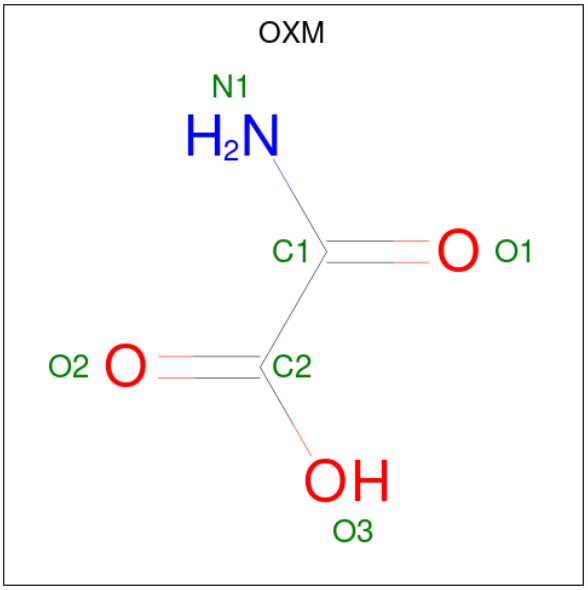
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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		

- Molecule 4 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	81	Total O 81 81	0	0
5	B	70	Total O 70 70	0	0

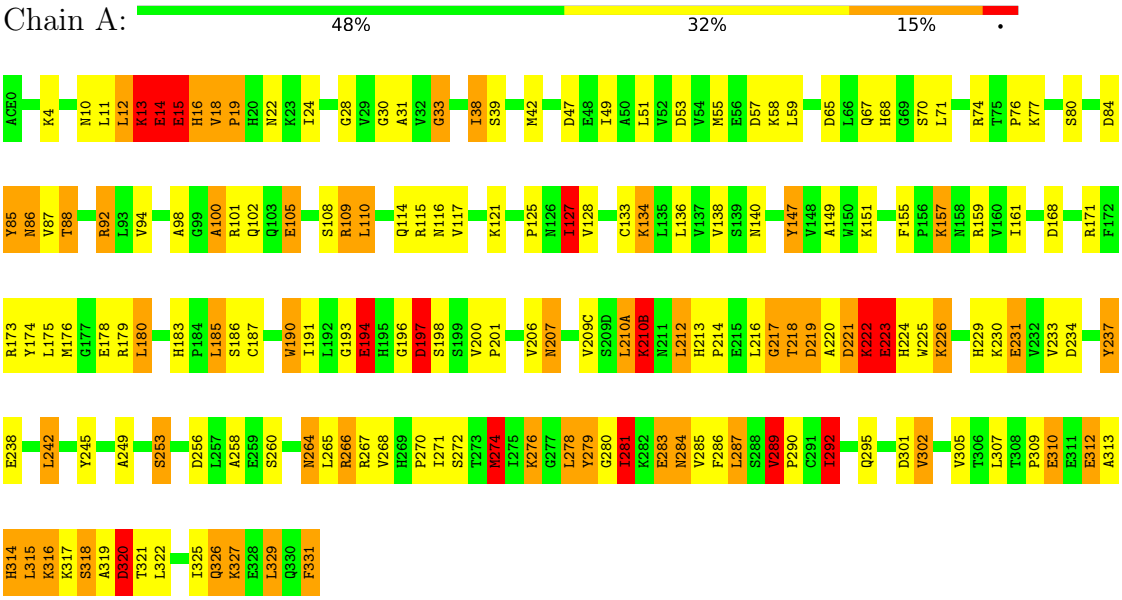
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

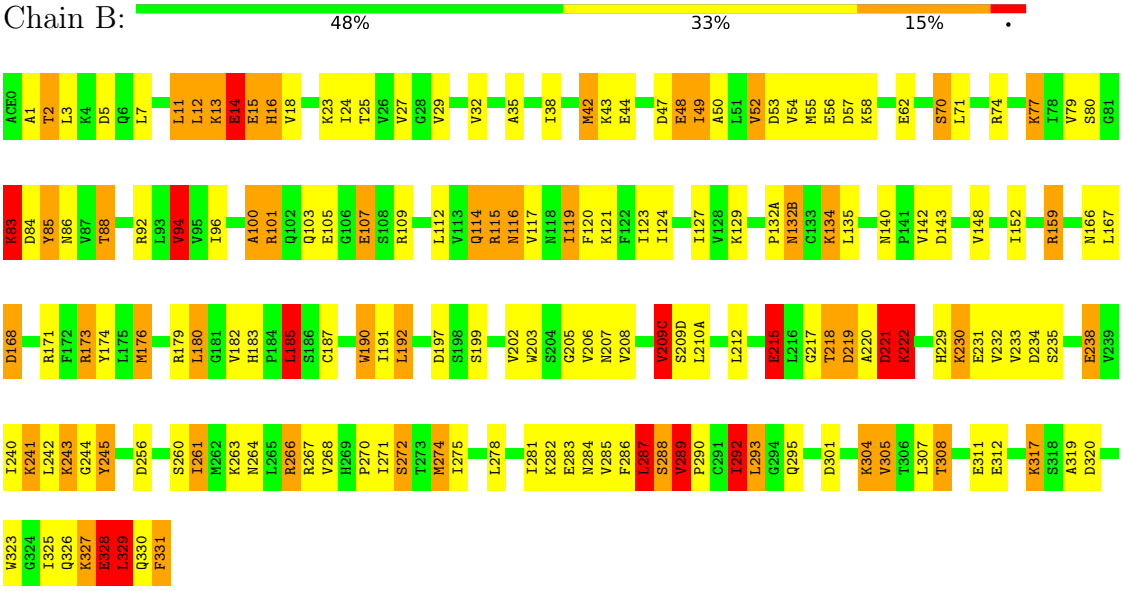
• Molecule 1: LACTATE DEHYDROGENASE

Chain A:



• Molecule 1: LACTATE DEHYDROGENASE

Chain B:



4 Data and refinement statistics (i)

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 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5396	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NAD, OXM, 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	1.14	5/2615 (0.2%)	2.55	164/3541 (4.6%)
1	B	1.13	4/2615 (0.2%)	2.55	164/3541 (4.6%)
All	All	1.14	9/5230 (0.2%)	2.55	328/7082 (4.6%)

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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	GLU	CD-OE2	7.98	1.34	1.25
1	B	14	GLU	CB-CG	7.52	1.66	1.52
1	A	74	ARG	CZ-NH2	7.18	1.42	1.33
1	B	238	GLU	CD-OE2	6.20	1.32	1.25
1	A	105	GLU	CD-OE2	5.41	1.31	1.25
1	A	196	GLY	N-CA	-5.32	1.38	1.46
1	A	178	GLU	CD-OE2	5.23	1.31	1.25
1	B	267	ARG	CZ-NH1	5.16	1.39	1.33
1	B	101	ARG	CD-NE	-5.07	1.37	1.46

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	ARG	NE-CZ-NH1	36.74	138.67	120.30
1	B	115	ARG	NE-CZ-NH2	29.63	135.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	ARG	NE-CZ-NH2	-24.70	107.95	120.30
1	B	221	ASP	C-N-CA	23.30	179.95	121.70
1	B	267	ARG	NE-CZ-NH1	-21.78	109.41	120.30
1	B	109	ARG	CD-NE-CZ	17.95	148.74	123.60
1	B	101	ARG	CD-NE-CZ	16.47	146.66	123.60
1	B	101	ARG	CG-CD-NE	16.37	146.19	111.80
1	B	15	GLU	CA-CB-CG	16.20	149.04	113.40
1	B	115	ARG	NE-CZ-NH1	-16.19	112.20	120.30
1	B	11	LEU	CA-CB-CG	16.18	152.52	115.30
1	B	197	ASP	CB-CG-OD2	-15.67	104.19	118.30
1	A	171	ARG	NE-CZ-NH1	-15.43	112.58	120.30
1	B	292	ILE	CA-CB-CG2	14.56	140.01	110.90
1	B	12	LEU	CA-CB-CG	14.44	148.52	115.30
1	A	237	TYR	CB-CG-CD2	-14.24	112.46	121.00
1	A	179	ARG	NE-CZ-NH1	-14.12	113.24	120.30
1	A	179	ARG	NE-CZ-NH2	13.88	127.24	120.30
1	A	212	LEU	CA-CB-CG	13.84	147.13	115.30
1	A	301	ASP	CB-CG-OD1	13.29	130.26	118.30
1	B	179	ARG	CD-NE-CZ	12.83	141.57	123.60
1	A	267	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	A	173	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	221	ASP	O-C-N	-11.46	104.37	122.70
1	A	256	ASP	CB-CG-OD2	-11.33	108.10	118.30
1	A	331	PHE	CB-CA-C	11.32	133.04	110.40
1	A	101	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	B	241	LYS	CA-CB-CG	10.97	137.53	113.40
1	A	272	SER	N-CA-CB	10.80	126.70	110.50
1	A	283	GLU	OE1-CD-OE2	10.76	136.21	123.30
1	A	266	ARG	NE-CZ-NH2	-10.53	115.04	120.30
1	B	267	ARG	NH1-CZ-NH2	10.49	130.94	119.40
1	B	221	ASP	CB-CG-OD1	10.18	127.46	118.30
1	A	237	TYR	CB-CG-CD1	10.07	127.04	121.00
1	A	312	GLU	OE1-CD-OE2	-9.83	111.50	123.30
1	A	174	TYR	CB-CG-CD1	-9.69	115.19	121.00
1	B	317	LYS	CA-CB-CG	9.65	134.63	113.40
1	A	55	MET	CG-SD-CE	-9.63	84.78	100.20
1	A	115	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	42	MET	CG-SD-CE	-9.59	84.86	100.20
1	A	301	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	B	92	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	B	301	ASP	CB-CG-OD1	9.46	126.82	118.30
1	A	256	ASP	CB-CG-OD1	9.37	126.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	256	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	B	266	ARG	CD-NE-CZ	9.20	136.47	123.60
1	B	44	GLU	OE1-CD-OE2	-9.14	112.33	123.30
1	A	196	GLY	N-CA-C	9.00	135.60	113.10
1	A	105	GLU	CB-CG-CD	8.99	138.48	114.20
1	A	53	ASP	CB-CG-OD2	8.99	126.39	118.30
1	A	74	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	65	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	B	14	GLU	CA-C-O	8.76	138.50	120.10
1	B	74	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	B	119	ILE	CA-CB-CG2	8.69	128.28	110.90
1	A	267	ARG	NH1-CZ-NH2	8.47	128.72	119.40
1	A	231	GLU	OE1-CD-OE2	-8.42	113.19	123.30
1	A	231	GLU	CA-CB-CG	8.39	131.85	113.40
1	A	274	MET	CA-CB-CG	-8.38	99.06	113.30
1	B	92	ARG	CD-NE-CZ	-8.31	111.96	123.60
1	A	219	ASP	CB-CG-OD1	-8.26	110.86	118.30
1	B	143	ASP	CB-CG-OD1	8.26	125.73	118.30
1	B	105	GLU	CG-CD-OE2	-8.14	102.03	118.30
1	A	84	ASP	CB-CG-OD1	-8.14	110.98	118.30
1	B	88	THR	N-CA-CB	-8.13	94.85	110.30
1	B	55	MET	CG-SD-CE	-8.09	87.26	100.20
1	A	276	LYS	CA-CB-CG	8.08	131.17	113.40
1	B	62	GLU	OE1-CD-OE2	-8.07	113.62	123.30
1	A	210(B)	LYS	CD-CE-NZ	7.97	130.03	111.70
1	A	92	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	A	77	LYS	N-CA-CB	7.96	124.92	110.60
1	B	289	VAL	CB-CA-C	7.90	126.41	111.40
1	A	179	ARG	CD-NE-CZ	7.87	134.61	123.60
1	B	35	ALA	N-CA-CB	7.76	120.96	110.10
1	B	176	MET	CG-SD-CE	-7.76	87.79	100.20
1	B	328	GLU	CA-CB-CG	7.69	130.33	113.40
1	A	115	ARG	NH1-CZ-NH2	7.61	127.78	119.40
1	A	221	ASP	CB-CG-OD1	7.61	125.15	118.30
1	B	109	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	B	232	VAL	CA-CB-CG1	7.56	122.24	110.90
1	B	266	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	B	272	SER	O-C-N	7.53	134.75	122.70
1	B	48	GLU	CA-CB-CG	7.53	129.96	113.40
1	A	266	ARG	NH1-CZ-NH2	7.51	127.66	119.40
1	B	292	ILE	CB-CA-C	7.51	126.62	111.60
1	B	320	ASP	CB-CG-OD2	7.51	125.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ILE	CB-CA-C	7.46	126.53	111.60
1	A	249	ALA	CB-CA-C	7.42	121.23	110.10
1	B	233	VAL	C-N-CA	7.41	140.22	121.70
1	A	87	VAL	CA-CB-CG2	7.39	121.98	110.90
1	A	178	GLU	CB-CG-CD	7.36	134.08	114.20
1	A	109	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	B	243	LYS	CA-C-O	-7.33	104.71	120.10
1	B	48	GLU	OE1-CD-OE2	-7.27	114.57	123.30
1	B	234	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	110	LEU	CB-CA-C	7.24	123.96	110.20
1	B	85	TYR	N-CA-CB	7.23	123.62	110.60
1	B	168	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	105	GLU	CG-CD-OE1	7.20	132.71	118.30
1	B	292	ILE	CB-CG1-CD1	-7.19	93.76	113.90
1	A	92	ARG	CD-NE-CZ	-7.19	113.53	123.60
1	A	197	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	176	MET	CG-SD-CE	-7.17	88.73	100.20
1	A	13	LYS	CA-CB-CG	7.13	129.09	113.40
1	A	115	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	B	283	GLU	OE1-CD-OE2	7.10	131.82	123.30
1	A	278	LEU	CB-CG-CD2	-7.06	99.00	111.00
1	A	171	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	121	LYS	CA-CB-CG	6.99	128.78	113.40
1	A	147	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	A	85	TYR	CB-CG-CD1	6.96	125.18	121.00
1	A	157	LYS	CA-CB-CG	6.95	128.70	113.40
1	B	35	ALA	O-C-N	6.92	133.77	122.70
1	B	14	GLU	CA-C-N	-6.92	101.99	117.20
1	B	284	ASN	CA-CB-CG	6.91	128.61	113.40
1	A	292	ILE	CA-CB-CG2	6.91	124.72	110.90
1	B	221	ASP	N-CA-CB	-6.91	98.17	110.60
1	A	171	ARG	CD-NE-CZ	-6.89	113.95	123.60
1	A	108	SER	CB-CA-C	6.87	123.14	110.10
1	A	220	ALA	CA-C-O	-6.87	105.68	120.10
1	A	267	ARG	CD-NE-CZ	-6.85	114.02	123.60
1	A	249	ALA	N-CA-CB	-6.84	100.52	110.10
1	B	219	ASP	CB-CA-C	6.84	124.08	110.40
1	A	86	ASN	CB-CG-OD1	-6.82	107.96	121.60
1	A	173	ARG	NH1-CZ-NH2	6.81	126.90	119.40
1	B	274	MET	CG-SD-CE	-6.80	89.32	100.20
1	A	222	LYS	CA-C-O	6.80	134.37	120.10
1	B	245	TYR	CB-CG-CD2	6.78	125.07	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	185	LEU	CA-CB-CG	6.76	130.84	115.30
1	A	14	GLU	CG-CD-OE2	-6.75	104.80	118.30
1	B	5	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	267	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	77	LYS	CA-CB-CG	6.71	128.16	113.40
1	B	173	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	310	GLU	CG-CD-OE2	-6.68	104.95	118.30
1	A	70	SER	CA-CB-OG	-6.66	93.21	111.20
1	B	29	VAL	CA-CB-CG1	6.65	120.87	110.90
1	A	278	LEU	CA-C-N	6.64	131.81	117.20
1	A	287	LEU	CB-CA-C	6.63	122.80	110.20
1	A	121	LYS	CA-CB-CG	6.62	127.97	113.40
1	A	289	VAL	N-CA-CB	-6.59	96.99	111.50
1	B	74	ARG	CG-CD-NE	6.59	125.64	111.80
1	A	253	SER	CA-C-N	6.59	131.69	117.20
1	A	38	ILE	CA-CB-CG2	6.55	124.01	110.90
1	B	159	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	B	43	LYS	C-N-CA	6.54	138.04	121.70
1	B	112	LEU	CB-CG-CD2	-6.52	99.92	111.00
1	A	217	GLY	C-N-CA	6.49	137.93	121.70
1	B	256	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	242	LEU	CA-CB-CG	6.44	130.11	115.30
1	A	127	ILE	CA-CB-CG2	6.42	123.74	110.90
1	A	147	TYR	CB-CG-CD1	6.41	124.84	121.00
1	A	264	ASN	CB-CG-OD1	6.41	134.42	121.60
1	B	219	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	260	SER	N-CA-CB	6.39	120.08	110.50
1	B	48	GLU	N-CA-CB	6.39	122.09	110.60
1	B	116	ASN	CB-CA-C	6.38	123.16	110.40
1	B	203	TRP	N-CA-CB	6.38	122.08	110.60
1	A	16	HIS	O-C-N	6.38	132.90	122.70
1	A	260	SER	N-CA-CB	6.37	120.05	110.50
1	A	312	GLU	CG-CD-OE1	6.35	131.01	118.30
1	B	159	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	289	VAL	CA-CB-CG1	6.33	120.40	110.90
1	A	77	LYS	O-C-N	6.32	132.82	122.70
1	B	221	ASP	CA-C-N	6.32	131.10	117.20
1	A	101	ARG	CD-NE-CZ	6.29	132.40	123.60
1	B	114	GLN	CB-CG-CD	6.29	127.94	111.60
1	A	84	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	13	LYS	CA-C-O	6.27	133.27	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	A	307	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	107	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	B	119	ILE	CB-CG1-CD1	-6.19	96.57	113.90
1	B	328	GLU	CB-CG-CD	6.19	130.91	114.20
1	B	38	ILE	CG1-CB-CG2	-6.19	97.79	111.40
1	B	115	ARG	NH1-CZ-NH2	-6.18	112.60	119.40
1	B	114	GLN	CA-CB-CG	6.16	126.95	113.40
1	B	83	LYS	N-CA-CB	6.16	121.68	110.60
1	B	166	ASN	CB-CG-ND2	6.15	131.46	116.70
1	B	14	GLU	CB-CG-CD	6.13	130.74	114.20
1	A	207	ASN	O-C-N	6.12	132.48	122.70
1	A	327	LYS	N-CA-CB	6.12	121.61	110.60
1	A	266	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	134	LYS	N-CA-CB	6.07	121.52	110.60
1	B	238	GLU	CA-C-N	6.07	130.55	117.20
1	B	168	ASP	O-C-N	6.05	132.38	122.70
1	B	287	LEU	CB-CA-C	6.05	121.69	110.20
1	B	261	ILE	CA-C-N	6.03	130.47	117.20
1	A	74	ARG	NH1-CZ-NH2	6.03	126.03	119.40
1	B	289	VAL	N-CA-CB	-6.02	98.25	111.50
1	A	245	TYR	CB-CG-CD2	6.01	124.61	121.00
1	A	149	ALA	CB-CA-C	5.98	119.08	110.10
1	A	194	GLU	OE1-CD-OE2	5.98	130.47	123.30
1	A	42	MET	CA-CB-CG	-5.95	103.19	113.30
1	B	307	LEU	O-C-N	5.95	132.22	122.70
1	A	194	GLU	CA-CB-CG	5.95	126.48	113.40
1	A	223	GLU	C-N-CA	5.93	136.53	121.70
1	B	261	ILE	O-C-N	-5.93	113.21	122.70
1	B	192	LEU	N-CA-CB	-5.92	98.55	110.40
1	B	312	GLU	CG-CD-OE2	-5.92	106.46	118.30
1	B	205	GLY	CA-C-O	-5.91	109.96	120.60
1	A	86	ASN	CA-CB-CG	5.90	126.37	113.40
1	B	84	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	A	285	VAL	CA-CB-CG1	5.88	119.73	110.90
1	B	2	THR	CA-CB-CG2	5.85	120.59	112.40
1	B	84	ASP	CA-C-N	5.85	130.07	117.20
1	A	197	ASP	N-CA-CB	-5.84	100.09	110.60
1	A	47	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	13	LYS	CA-C-N	-5.81	104.41	117.20
1	A	77	LYS	CB-CG-CD	5.81	126.72	111.60
1	A	88	THR	CA-CB-CG2	5.81	120.54	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	GLU	CB-CA-C	-5.81	98.78	110.40
1	B	180	LEU	CB-CG-CD2	-5.81	101.13	111.00
1	B	185	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	220	ALA	CB-CA-C	5.80	118.80	110.10
1	B	86	ASN	CB-CG-ND2	5.79	130.60	116.70
1	A	310	GLU	CG-CD-OE1	5.78	129.86	118.30
1	B	301	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	65	ASP	CA-C-O	-5.76	108.01	120.10
1	B	29	VAL	CG1-CB-CG2	-5.75	101.70	110.90
1	B	270	PRO	CA-C-O	-5.74	106.42	120.20
1	B	263	LYS	CD-CE-NZ	-5.74	98.51	111.70
1	B	190	TRP	O-C-N	5.73	131.87	122.70
1	A	57	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	312	GLU	CA-CB-CG	5.71	125.96	113.40
1	B	14	GLU	C-N-CA	5.70	135.94	121.70
1	B	209(C)	VAL	CB-CA-C	5.69	122.21	111.40
1	B	320	ASP	OD1-CG-OD2	-5.68	112.50	123.30
1	A	190	TRP	CD1-CG-CD2	-5.68	101.76	106.30
1	A	176	MET	CB-CA-C	5.68	121.75	110.40
1	A	168	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	B	327	LYS	C-N-CA	5.66	135.86	121.70
1	B	230	LYS	CD-CE-NZ	5.66	124.71	111.70
1	B	222	LYS	CB-CA-C	-5.65	99.10	110.40
1	A	105	GLU	CG-CD-OE1	5.65	129.60	118.30
1	A	318	SER	CB-CA-C	-5.65	99.37	110.10
1	A	278	LEU	CA-C-O	-5.64	108.26	120.10
1	A	253	SER	CB-CA-C	5.63	120.79	110.10
1	A	86	ASN	CB-CA-C	5.62	121.63	110.40
1	B	42	MET	CA-CB-CG	-5.60	103.78	113.30
1	B	210(A)	LEU	CB-CA-C	5.60	120.84	110.20
1	A	67	GLN	C-N-CA	5.59	135.67	121.70
1	B	84	ASP	N-CA-C	5.59	126.08	111.00
1	B	304	LYS	CB-CG-CD	5.57	126.07	111.60
1	A	176	MET	N-CA-CB	-5.52	100.66	110.60
1	A	289	VAL	CB-CA-C	5.51	121.87	111.40
1	A	92	ARG	NH1-CZ-NH2	-5.50	113.34	119.40
1	A	187	CYS	N-CA-CB	5.50	120.51	110.60
1	A	155	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	B	221	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	159	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	B	70	SER	CB-CA-C	-5.49	99.68	110.10
1	A	174	TYR	CB-CG-CD2	5.47	124.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ASP	OD1-CG-OD2	5.46	133.67	123.30
1	A	279	TYR	CB-CA-C	5.46	121.31	110.40
1	B	16	HIS	CA-CB-CG	-5.45	104.34	113.60
1	B	190	TRP	CA-C-N	-5.45	105.22	117.20
1	B	305	VAL	CB-CA-C	5.44	121.74	111.40
1	B	327	LYS	O-C-N	-5.44	114.00	122.70
1	B	222	LYS	N-CA-C	5.43	125.65	111.00
1	B	243	LYS	N-CA-CB	5.42	120.36	110.60
1	B	179	ARG	NH1-CZ-NH2	-5.41	113.44	119.40
1	A	16	HIS	CB-CA-C	5.40	121.20	110.40
1	A	12	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	59	LEU	O-C-N	5.38	131.31	122.70
1	A	281	ILE	N-CA-C	-5.38	96.47	111.00
1	B	53	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	117	VAL	CA-C-N	5.37	129.01	117.20
1	A	225	TRP	O-C-N	5.37	131.29	122.70
1	B	243	LYS	O-C-N	5.36	132.31	123.20
1	B	288	SER	CA-C-N	-5.36	105.41	117.20
1	B	44	GLU	CG-CD-OE1	5.35	129.00	118.30
1	A	125	PRO	N-CA-CB	5.35	109.72	103.30
1	A	197	ASP	CA-CB-CG	5.34	125.15	113.40
1	B	70	SER	CA-CB-OG	-5.33	96.80	111.20
1	A	74	ARG	CG-CD-NE	5.33	123.00	111.80
1	A	267	ARG	CB-CG-CD	-5.33	97.75	111.60
1	A	33	GLY	CA-C-O	-5.31	111.03	120.60
1	A	268	VAL	CA-CB-CG1	5.31	118.87	110.90
1	B	312	GLU	CG-CD-OE1	5.31	128.92	118.30
1	B	197	ASP	OD1-CG-OD2	5.31	133.39	123.30
1	B	100	ALA	O-C-N	5.28	131.14	122.70
1	B	101	ARG	O-C-N	-5.27	114.27	122.70
1	B	80	SER	N-CA-CB	-5.26	102.60	110.50
1	A	98	ALA	N-CA-CB	-5.26	102.73	110.10
1	B	263	LYS	CA-C-O	-5.25	109.07	120.10
1	A	68	HIS	N-CA-CB	5.24	120.03	110.60
1	A	234	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	B	57	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	292	ILE	CG1-CB-CG2	-5.21	99.93	111.40
1	A	229	HIS	N-CA-CB	5.20	119.96	110.60
1	B	103	GLN	N-CA-C	-5.19	96.99	111.00
1	A	326	GLN	CA-C-O	-5.18	109.22	120.10
1	B	159	ARG	CD-NE-CZ	5.18	130.85	123.60
1	B	215	GLU	OE1-CD-OE2	5.18	129.52	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	174	TYR	CB-CG-CD1	-5.17	117.89	121.00
1	A	320	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	47	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	152	ILE	CA-CB-CG1	5.17	120.82	111.00
1	B	274	MET	N-CA-CB	-5.16	101.31	110.60
1	B	107	GLU	CG-CD-OE1	5.16	128.61	118.30
1	A	258	ALA	N-CA-CB	5.15	117.31	110.10
1	B	94	VAL	CA-CB-CG1	5.13	118.60	110.90
1	B	220	ALA	C-N-CA	5.12	134.50	121.70
1	B	268	VAL	CA-CB-CG1	5.12	118.58	110.90
1	A	180	LEU	N-CA-CB	-5.12	100.16	110.40
1	A	101	ARG	N-CA-CB	5.11	119.81	110.60
1	B	241	LYS	CG-CD-CE	5.11	127.22	111.90
1	A	292	ILE	CB-CA-C	5.11	121.81	111.60
1	B	272	SER	N-CA-CB	5.10	118.15	110.50
1	B	222	LYS	N-CA-CB	5.09	119.76	110.60
1	B	179	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	174	TYR	CB-CG-CD2	5.07	124.04	121.00
1	A	302	VAL	O-C-N	-5.07	114.59	122.70
1	A	186	SER	CA-C-O	-5.07	109.46	120.10
1	A	101	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	108	SER	CA-CB-OG	5.05	124.84	111.20
1	B	134	LYS	N-CA-CB	5.04	119.68	110.60
1	A	309	PRO	O-C-N	5.04	130.76	122.70
1	B	218	THR	C-N-CA	5.03	134.27	121.70
1	A	100	ALA	O-C-N	5.03	130.74	122.70
1	B	71	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	B	94	VAL	CB-CA-C	5.02	120.94	111.40
1	B	287	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	14	GLU	OE1-CD-OE2	5.01	129.32	123.30
1	A	245	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	B	191	ILE	N-CA-CB	5.01	122.33	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Sidechain
1	A	265	LEU	Mainchain

5.2 Too-close contacts (i)

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	87	0
1	B	2568	0	2641	89	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	44	0	26	3	0
3	B	44	0	26	1	0
4	B	6	0	2	0	0
5	A	81	0	0	6	1
5	B	70	0	0	9	1
All	All	5396	0	5337	169	2

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 16.

All (169) 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:B:217:GLY:O	1:B:219:ASP:N	1.93	1.01
1:A:221:ASP:O	1:A:222:LYS:HB2	1.58	0.99
1:B:13:LYS:CG	1:B:14:GLU:H	1.82	0.91
1:B:290:PRO:HG2	1:B:305:VAL:HG11	1.53	0.90
1:B:100:ALA:H	1:B:116:ASN:HD21	1.18	0.89
1:A:100:ALA:H	1:A:116:ASN:HD21	0.93	0.88
1:A:100:ALA:N	1:A:116:ASN:HD21	1.75	0.84
1:B:114:GLN:HG3	1:B:330:GLN:HE22	1.45	0.82
1:B:308:THR:HG22	1:B:311:GLU:HG3	1.60	0.82
1:A:161:ILE:HG23	1:A:271:ILE:HD12	1.60	0.81
1:B:275:ILE:CD1	1:B:281:ILE:HG13	2.13	0.79
1:B:217:GLY:C	1:B:219:ASP:H	1.86	0.77
1:B:13:LYS:HG3	1:B:14:GLU:H	1.48	0.77
1:A:210(A):LEU:HD11	1:B:7:LEU:HD22	1.67	0.76
1:A:222:LYS:HG2	1:A:223:GLU:H	1.51	0.76
1:A:100:ALA:H	1:A:116:ASN:ND2	1.77	0.75
1:B:132(B):ASN:HA	1:B:159:ARG:NH1	2.02	0.75
1:A:193:GLY:HA2	1:A:287:LEU:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LYS:HB2	1:A:283:GLU:O	1.89	0.73
1:B:266:ARG:HB3	1:B:292:ILE:HD11	1.69	0.73
1:A:85:TYR:O	1:A:88:THR:HB	1.88	0.73
1:B:238:GLU:O	1:B:242:LEU:HD12	1.88	0.72
1:B:77:LYS:HE3	5:B:454:HOH:O	1.90	0.71
1:A:4:LYS:HG2	5:B:406:HOH:O	1.91	0.70
1:B:132(A):PRO:O	1:B:159:ARG:NH1	2.23	0.70
1:A:4:LYS:CG	5:B:406:HOH:O	2.39	0.69
5:A:481:HOH:O	1:B:2:THR:HG22	1.93	0.69
1:A:4:LYS:HE3	5:A:439:HOH:O	1.91	0.69
1:A:161:ILE:CG2	1:A:271:ILE:HD12	2.23	0.68
1:B:285:VAL:HG21	1:B:319:ALA:HB1	1.75	0.68
1:B:274:MET:HG2	1:B:286:PHE:CE2	2.28	0.67
1:A:289:VAL:HG13	1:A:302:VAL:HG13	1.76	0.67
1:A:10:ASN:ND2	1:A:12:LEU:O	2.29	0.66
1:B:271:ILE:O	1:B:288:SER:HA	1.96	0.65
1:B:114:GLN:HG3	1:B:330:GLN:NE2	2.11	0.65
1:B:290:PRO:HG2	1:B:305:VAL:CG1	2.25	0.65
1:B:123:ILE:HG13	1:B:124:ILE:N	2.12	0.64
1:B:117:VAL:HG22	1:B:148:VAL:HG21	1.79	0.64
1:B:243:LYS:HE2	1:B:245:TYR:O	1.97	0.64
1:A:221:ASP:O	1:A:222:LYS:CB	2.43	0.63
1:B:100:ALA:N	1:B:116:ASN:HD21	1.94	0.63
1:A:14:GLU:C	1:A:15:GLU:O	2.35	0.63
1:B:13:LYS:CG	1:B:14:GLU:N	2.60	0.62
1:A:281:ILE:C	1:A:281:ILE:HD13	2.21	0.61
1:A:175:LEU:HD13	1:A:231:GLU:HG3	1.82	0.61
1:A:198:SER:O	1:A:318:SER:OG	2.17	0.61
1:A:266:ARG:HB3	1:A:292:ILE:HD13	1.82	0.61
1:A:264:ASN:HB2	1:A:295:GLN:HB3	1.83	0.61
1:A:190:TRP:CZ3	1:A:270:PRO:HD3	2.35	0.61
1:B:88:THR:CG2	5:B:451:HOH:O	2.48	0.60
1:B:190:TRP:HB3	1:B:192:LEU:HD13	1.83	0.60
1:A:22:ASN:ND2	1:A:92:ARG:HH21	2.01	0.59
1:B:176:MET:HE1	1:B:206:VAL:HG11	1.84	0.59
1:A:22:ASN:HD22	1:A:92:ARG:HH21	1.50	0.59
1:A:314:HIS:HB3	5:A:414:HOH:O	2.02	0.58
1:A:289:VAL:CG1	1:A:302:VAL:HG13	2.32	0.58
1:B:183:HIS:ND1	1:B:185:LEU:HB2	2.19	0.58
1:A:127:ILE:HD11	1:A:133:CYS:SG	2.43	0.58
1:A:289:VAL:HG13	1:A:302:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG21	1:A:127:ILE:HD13	1.85	0.58
1:B:266:ARG:HB3	1:B:292:ILE:CD1	2.33	0.57
1:B:176:MET:CE	1:B:206:VAL:HG11	2.35	0.56
1:A:140:ASN:HB2	3:A:401:NAD:O2D	2.06	0.56
1:B:274:MET:CG	1:B:286:PHE:CE2	2.89	0.56
1:A:197:ASP:HA	1:A:233:VAL:HG13	1.88	0.55
1:B:275:ILE:HG12	1:B:287:LEU:CD1	2.37	0.55
1:B:328:GLU:O	1:B:330:GLN:N	2.39	0.55
1:A:329:LEU:C	1:A:331:PHE:H	2.06	0.55
1:B:182:VAL:HG23	1:B:187:CYS:SG	2.47	0.55
1:A:183:HIS:ND1	1:A:185:LEU:HB2	2.22	0.55
1:B:120:PHE:HA	1:B:123:ILE:HG12	1.88	0.55
1:B:329:LEU:HA	1:B:331:PHE:CE1	2.42	0.55
1:A:71:LEU:HD12	1:B:185:LEU:HD13	1.89	0.54
1:B:182:VAL:CG2	1:B:187:CYS:SG	2.96	0.54
1:B:16:HIS:CG	1:B:16:HIS:O	2.60	0.54
1:A:210(B):LYS:NZ	1:A:214:PRO:O	2.41	0.53
1:B:13:LYS:CD	1:B:14:GLU:H	2.21	0.53
1:A:109:ARG:HG3	5:A:408:HOH:O	2.08	0.53
1:B:25:THR:HB	1:B:94:VAL:HB	1.90	0.53
1:B:127:ILE:HG21	1:B:135:LEU:HD21	1.91	0.52
1:A:51:LEU:O	1:A:80:SER:HA	2.09	0.52
1:B:275:ILE:HG12	1:B:287:LEU:HD11	1.92	0.52
1:A:15:GLU:OE1	1:A:18:VAL:HG12	2.10	0.52
1:B:199:SER:OG	1:B:229:HIS:HE1	1.93	0.52
1:A:138:VAL:O	3:A:401:NAD:H2N	2.10	0.51
1:A:213:HIS:HD2	1:A:216:LEU:HB2	1.75	0.51
1:A:213:HIS:NE2	1:A:222:LYS:HG3	2.25	0.51
1:A:222:LYS:HB3	1:A:224:HIS:H	1.75	0.51
1:A:279:TYR:N	1:A:281:ILE:HG22	2.25	0.51
1:B:32:VAL:HG21	3:B:401:NAD:C6N	2.40	0.51
1:B:115:ARG:HD3	5:B:419:HOH:O	2.11	0.51
1:B:275:ILE:HD12	1:B:281:ILE:HG13	1.91	0.51
1:A:4:LYS:HB3	5:B:406:HOH:O	2.11	0.51
1:A:222:LYS:CG	1:A:223:GLU:H	2.01	0.51
1:A:279:TYR:H	1:A:281:ILE:HG22	1.75	0.51
1:B:27:VAL:HG22	1:B:52:VAL:HG22	1.93	0.50
1:B:215:GLU:O	1:B:219:ASP:HB2	2.11	0.50
1:A:210(A):LEU:HD11	1:B:7:LEU:CD2	2.38	0.50
1:A:13:LYS:HB2	1:A:14:GLU:HG3	1.94	0.50
1:A:310:GLU:O	1:A:313:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASP:HB3	1:B:222:LYS:HD2	1.93	0.50
1:B:192:LEU:HD22	1:B:202:VAL:HG21	1.93	0.49
1:B:88:THR:HG23	5:B:451:HOH:O	2.10	0.49
1:A:39:SER:HA	1:B:42:MET:CE	2.42	0.49
1:B:13:LYS:HG3	1:B:14:GLU:N	2.25	0.49
1:A:289:VAL:CG1	1:A:302:VAL:CG1	2.91	0.48
1:A:206:VAL:HG12	1:A:210(A):LEU:HD22	1.94	0.48
1:A:320:ASP:O	1:A:321:THR:C	2.50	0.48
1:B:243:LYS:HE3	1:B:245:TYR:CE2	2.49	0.48
1:B:140:ASN:HA	1:B:142:VAL:N	2.29	0.48
1:A:14:GLU:O	1:A:16:HIS:HD2	1.97	0.48
1:B:275:ILE:HD12	1:B:281:ILE:HG21	1.96	0.48
1:B:275:ILE:HD13	1:B:281:ILE:HG13	1.93	0.48
1:A:38:ILE:HA	1:A:38:ILE:HD12	1.75	0.47
1:B:329:LEU:HA	1:B:331:PHE:HE1	1.79	0.47
1:A:110:LEU:HD13	1:A:325:ILE:CD1	2.44	0.47
1:A:13:LYS:O	1:A:15:GLU:N	2.48	0.47
1:B:96:ILE:HD11	1:B:135:LEU:HD22	1.96	0.46
1:B:275:ILE:HG12	1:B:287:LEU:HG	1.97	0.46
1:A:127:ILE:HG13	1:A:128:VAL:N	2.30	0.46
1:B:85:TYR:O	1:B:88:THR:HB	2.14	0.46
1:A:280:GLY:O	1:A:316:LYS:HE2	2.15	0.46
1:A:15:GLU:O	1:A:16:HIS:CD2	2.68	0.46
1:A:218:THR:HA	1:A:226:LYS:HE3	1.98	0.46
1:A:292:ILE:C	1:A:292:ILE:HD12	2.37	0.45
1:A:284:ASN:HB2	5:A:477:HOH:O	2.15	0.45
1:B:308:THR:CG2	1:B:311:GLU:HG3	2.40	0.45
1:A:18:VAL:CG2	1:A:19:PRO:HD2	2.45	0.45
1:A:39:SER:HA	1:B:42:MET:HE3	1.96	0.45
1:A:213:HIS:HB2	1:B:3:LEU:HD13	1.98	0.45
1:B:56:GLU:OE1	1:B:83:LYS:HE2	2.17	0.45
1:A:210(A):LEU:CD1	1:B:7:LEU:HD22	2.41	0.44
1:A:274:MET:HG3	1:A:286:PHE:CE2	2.52	0.44
1:B:50:ALA:HA	1:B:79:VAL:O	2.18	0.44
1:B:190:TRP:HB3	1:B:192:LEU:CD1	2.47	0.44
1:B:289:VAL:HA	1:B:290:PRO:HD3	1.78	0.44
1:B:173:ARG:NE	1:B:187:CYS:O	2.50	0.44
1:A:197:ASP:HA	1:A:233:VAL:CG1	2.47	0.44
1:B:23:LYS:HE3	1:B:48:GLU:OE2	2.18	0.43
1:A:287:LEU:HD21	1:A:319:ALA:HB2	2.00	0.43
1:B:208:VAL:O	1:B:209(C):VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:HD13	1:A:283:GLU:H	1.84	0.42
3:A:401:NAD:H6N	5:A:413:HOH:O	2.17	0.42
1:A:24:ILE:O	1:A:49:ILE:HA	2.19	0.42
1:A:28:GLY:O	1:A:33:GLY:HA3	2.19	0.42
1:B:24:ILE:O	1:B:49:ILE:HA	2.18	0.42
1:B:240:ILE:O	1:B:244:GLY:N	2.49	0.42
1:B:231:GLU:O	1:B:235:SER:HB3	2.20	0.42
1:B:77:LYS:HE2	5:B:455:HOH:O	2.20	0.41
1:B:286:PHE:O	1:B:287:LEU:HB3	2.19	0.41
1:B:271:ILE:CD1	1:B:293:LEU:HG	2.50	0.41
1:A:30:GLY:O	1:A:31:ALA:C	2.57	0.41
1:B:261:ILE:HG13	1:B:293:LEU:HD13	2.03	0.41
1:A:14:GLU:O	1:A:16:HIS:CD2	2.72	0.41
1:A:200:VAL:HG21	1:A:315:LEU:HD12	2.01	0.41
1:A:289:VAL:HA	1:A:290:PRO:HD3	1.91	0.41
1:B:285:VAL:HG12	1:B:326:GLN:NE2	2.36	0.41
1:B:264:ASN:HB2	1:B:295:GLN:HB3	2.01	0.41
1:B:167:LEU:O	1:B:171:ARG:HG3	2.20	0.41
1:A:194:GLU:HG3	1:A:322:LEU:HD22	2.01	0.41
1:A:102:GLN:CD	1:A:109:ARG:HG2	2.41	0.41
1:A:191:ILE:CD1	1:A:201:PRO:HA	2.52	0.41
1:B:266:ARG:CB	1:B:292:ILE:HD11	2.45	0.41
1:B:107:GLU:OE1	5:B:473:HOH:O	2.22	0.40
1:A:85:TYR:CE2	1:A:127:ILE:HG22	2.56	0.40
1:A:147:TYR:CD2	1:A:326:GLN:HG2	2.56	0.40
1:A:212:LEU:HD12	1:B:3:LEU:HD12	2.04	0.40
1:A:217:GLY:H	1:A:222:LYS:NZ	2.19	0.40
1:A:279:TYR:H	1:A:281:ILE:CG2	2.35	0.40

All (2) 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)
5:A:483:HOH:O	5:B:473:HOH:O[4_455]	1.28	0.92
1:B:132(B):ASN:OD1	1:B:132(B):ASN:OD1[2_655]	1.63	0.57

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	330/332 (99%)	302 (92%)	22 (7%)	6 (2%)	8 5
1	B	330/332 (99%)	309 (94%)	14 (4%)	7 (2%)	7 4
All	All	660/664 (99%)	611 (93%)	36 (6%)	13 (2%)	7 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	218	THR
1	A	222	LYS
1	B	1	ALA
1	B	14	GLU
1	B	218	THR
1	B	222	LYS
1	B	329	LEU
1	A	219	ASP
1	A	329	LEU
1	A	15	GLU
1	B	15	GLU
1	B	328	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	285/285 (100%)	242 (85%)	43 (15%)	3 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	285/285 (100%)	240 (84%)	45 (16%)	2 2
All	All	570/570 (100%)	482 (85%)	88 (15%)	2 2

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	LYS
1	A	14	GLU
1	A	15	GLU
1	A	18	VAL
1	A	19	PRO
1	A	58	LYS
1	A	76	PRO
1	A	86	ASN
1	A	105	GLU
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	180	LEU
1	A	194	GLU
1	A	197	ASP
1	A	207	ASN
1	A	209(C)	VAL
1	A	210(A)	LEU
1	A	210(B)	LYS
1	A	222	LYS
1	A	223	GLU
1	A	226	LYS
1	A	230	LYS
1	A	242	LEU
1	A	253	SER
1	A	274	MET
1	A	278	LEU
1	A	281	ILE
1	A	284	ASN
1	A	289	VAL
1	A	292	ILE
1	A	305	VAL

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	314	HIS
1	A	315	LEU
1	A	316	LYS
1	A	317	LYS
1	A	320	ASP
1	A	327	LYS
1	B	11	LEU
1	B	12	LEU
1	B	13	LYS
1	B	14	GLU
1	B	18	VAL
1	B	49	ILE
1	B	52	VAL
1	B	54	VAL
1	B	58	LYS
1	B	70	SER
1	B	77	LYS
1	B	83	LYS
1	B	94	VAL
1	B	101	ARG
1	B	119	ILE
1	B	129	LYS
1	B	132(B)	ASN
1	B	134	LYS
1	B	168	ASP
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	221	ASP
1	B	230	LYS
1	B	241	LYS
1	B	272	SER
1	B	278	LEU
1	B	282	LYS
1	B	287	LEU
1	B	289	VAL
1	B	292	ILE

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	304	LYS
1	B	308	THR
1	B	317	LYS
1	B	323	TRP
1	B	325	ILE
1	B	327	LYS
1	B	328	GLU
1	B	329	LEU
1	B	331	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	16	HIS
1	A	22	ASN
1	A	116	ASN
1	A	229	HIS
1	A	284	ASN
1	B	116	ASN
1	B	207	ASN
1	B	229	HIS
1	B	330	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	42,48,48	1.47	4 (9%)	50,73,73	2.59	19 (38%)
2	SO4	A	402	-	4,4,4	0.73	0	6,6,6	2.47	4 (66%)
4	OXM	B	402	-	5,5,5	8.75	4 (80%)	4,6,6	8.38	3 (75%)
2	SO4	B	403	-	4,4,4	0.71	0	6,6,6	0.91	0
3	NAD	B	401	-	42,48,48	1.33	3 (7%)	50,73,73	2.65	19 (38%)
2	SO4	A	403	-	4,4,4	0.89	0	6,6,6	0.70	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	B	401	-	-	4/26/62/62	0/5/5/5
3	NAD	A	401	-	-	4/26/62/62	0/5/5/5
4	OXM	B	402	-	-	0/3/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	OXM	C1-C2	-14.23	1.37	1.55
4	B	402	OXM	C1-N1	11.82	1.65	1.33
3	A	401	NAD	C3N-C7N	5.77	1.59	1.50
4	B	402	OXM	O1-C1	5.22	1.36	1.24
3	B	401	NAD	C3N-C7N	4.71	1.57	1.50
4	B	402	OXM	O2-C2	3.72	1.32	1.22
3	B	401	NAD	C6N-N1N	3.42	1.43	1.35
3	B	401	NAD	O7N-C7N	-3.39	1.17	1.24
3	A	401	NAD	C6N-N1N	3.26	1.43	1.35
3	A	401	NAD	C2B-C1B	-2.79	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C2A-N3A	-2.69	1.27	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	OXM	O3-C2-C1	12.64	143.06	113.84
4	B	402	OXM	O2-C2-C1	-10.75	98.12	122.06
3	A	401	NAD	C5A-C6A-N6A	9.89	135.39	120.35
3	B	401	NAD	C5N-C4N-C3N	-7.88	111.01	120.34
3	B	401	NAD	C2N-C3N-C4N	6.42	125.53	118.26
3	B	401	NAD	O4D-C1D-C2D	-6.22	97.83	106.93
3	B	401	NAD	C6N-C5N-C4N	5.94	128.07	119.44
3	A	401	NAD	N6A-C6A-N1A	-5.42	107.33	118.57
3	A	401	NAD	C5N-C4N-C3N	-5.30	114.07	120.34
3	B	401	NAD	O4B-C1B-C2B	-4.92	99.73	106.93
3	A	401	NAD	O7N-C7N-N7N	4.53	129.01	122.58
3	A	401	NAD	C6N-C5N-C4N	4.36	125.78	119.44
3	A	401	NAD	C2N-C3N-C4N	4.18	123.00	118.26
3	B	401	NAD	O2B-C2B-C3B	3.94	124.56	111.82
2	A	402	SO4	O4-S-O1	3.93	129.80	109.31
3	B	401	NAD	C5A-C6A-N6A	3.83	126.18	120.35
3	B	401	NAD	C5N-C6N-N1N	-3.45	115.45	120.40
3	A	401	NAD	C1B-N9A-C4A	-3.44	120.60	126.64
3	A	401	NAD	C4N-C3N-C7N	-3.28	112.27	121.04
3	B	401	NAD	C6N-N1N-C2N	-3.19	119.06	121.97
3	A	401	NAD	C3N-C7N-N7N	-3.19	113.92	117.75
3	B	401	NAD	O2A-PA-O1A	3.18	127.96	112.24
2	A	402	SO4	O4-S-O3	-3.02	96.17	109.06
3	B	401	NAD	O7N-C7N-N7N	3.00	126.83	122.58
3	B	401	NAD	O5B-C5B-C4B	-2.92	98.95	108.99
3	B	401	NAD	O5D-PN-O1N	2.87	120.30	109.07
3	A	401	NAD	O2B-C2B-C3B	2.84	121.01	111.82
3	A	401	NAD	C5N-C6N-N1N	-2.79	116.40	120.40
3	A	401	NAD	O2N-PN-O5D	2.68	120.17	107.75
3	A	401	NAD	O5D-PN-O1N	2.44	118.62	109.07
2	A	402	SO4	O3-S-O2	2.42	121.92	109.31
3	A	401	NAD	O7N-C7N-C3N	-2.39	116.77	119.63
3	B	401	NAD	C4N-C3N-C7N	-2.39	114.64	121.04
3	A	401	NAD	C6N-N1N-C2N	-2.37	119.82	121.97
3	B	401	NAD	C1B-N9A-C4A	-2.33	122.55	126.64
2	A	402	SO4	O3-S-O1	-2.28	97.40	109.31
4	B	402	OXM	O3-C2-O2	-2.23	118.50	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	NAD	C3B-C2B-C1B	2.19	104.28	100.98
3	A	401	NAD	C4A-C5A-N7A	-2.17	107.14	109.40
3	B	401	NAD	O4D-C4D-C5D	-2.14	102.33	109.37
3	A	401	NAD	N3A-C2A-N1A	-2.13	125.35	128.68
3	B	401	NAD	O7N-C7N-C3N	-2.12	117.09	119.63
3	B	401	NAD	O3D-C3D-C4D	-2.11	104.96	111.05
3	A	401	NAD	C5B-C4B-C3B	-2.10	107.31	115.18
3	A	401	NAD	O2D-C2D-C3D	2.07	118.53	111.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	C2D-C1D-N1N-C6N
3	B	401	NAD	O4B-C4B-C5B-O5B
3	A	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	C2D-C1D-N1N-C2N
3	A	401	NAD	O4B-C4B-C5B-O5B

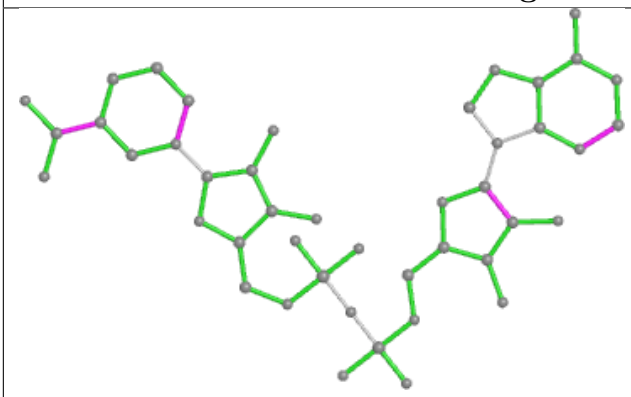
There are no ring outliers.

2 monomers are involved in 4 short contacts:

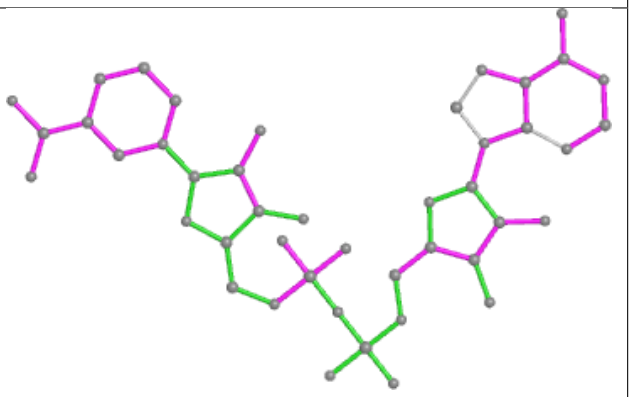
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAD	3	0
3	B	401	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

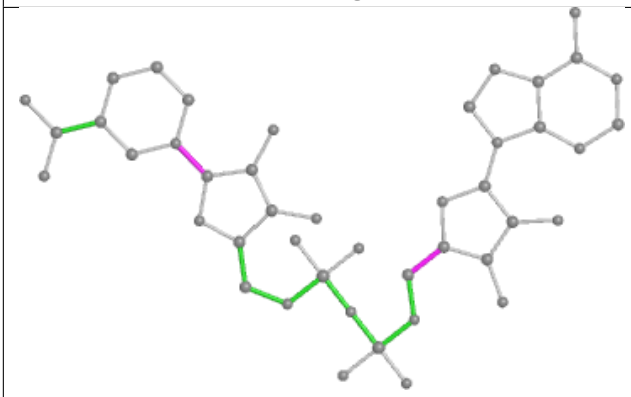
Ligand NAD A 401



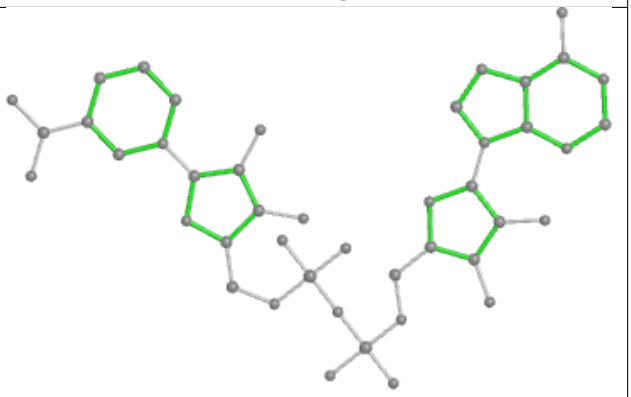
Bond lengths



Bond angles

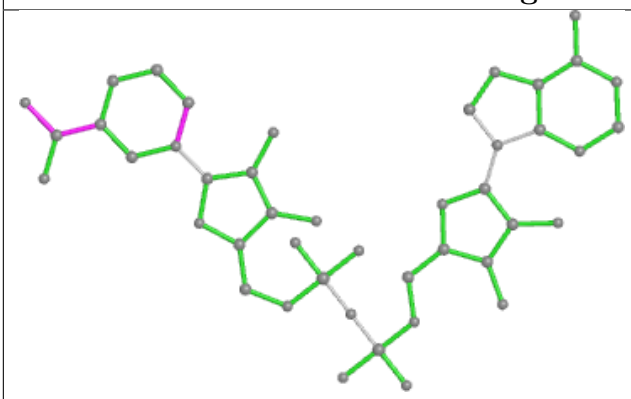


Torsions

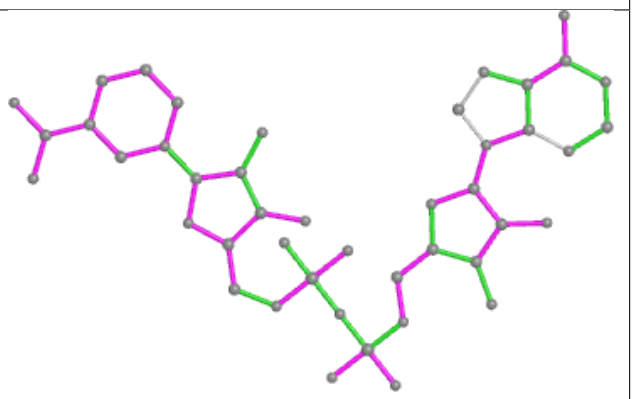


Rings

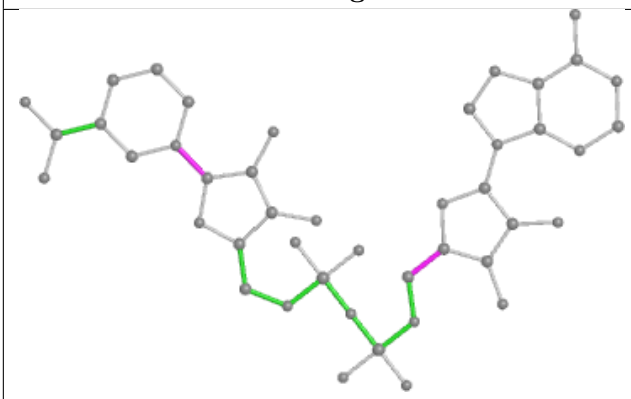
Ligand NAD B 401



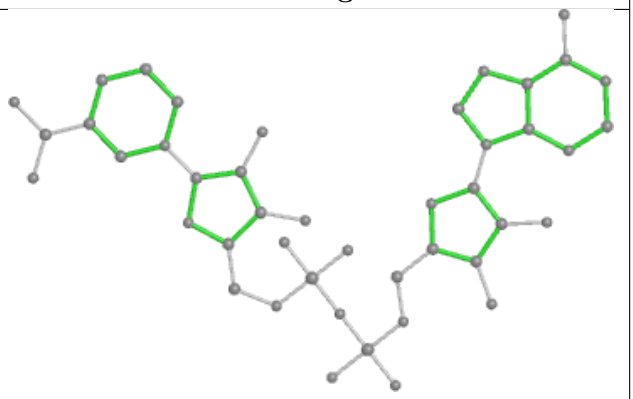
Bond lengths



Bond angles



Torsions



Rings

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.