Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:32 PM EDT

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	:	1991-11-26
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
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:

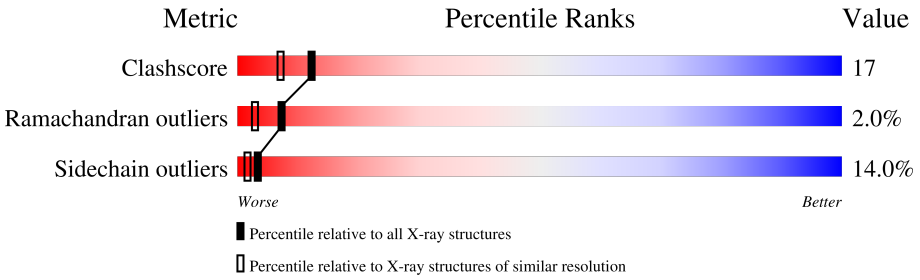
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	45% 34% 15% 6%
1	B	332	41% 36% 19% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OXM	A	402	-	X	-	-
4	OXM	B	402	-	X	-	-

2 Entry composition

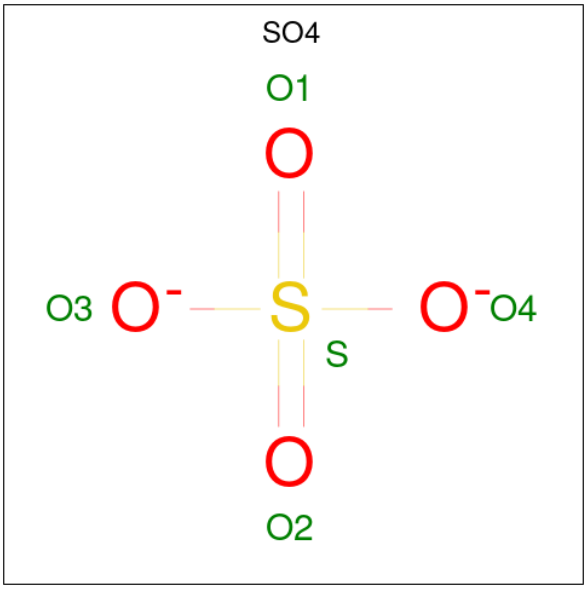
There are 5 unique types of molecules in this entry. The entry contains 5399 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

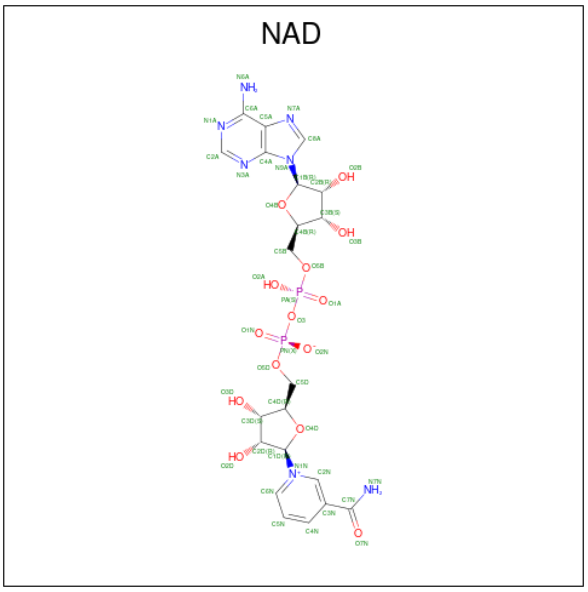
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			
1	B	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			

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



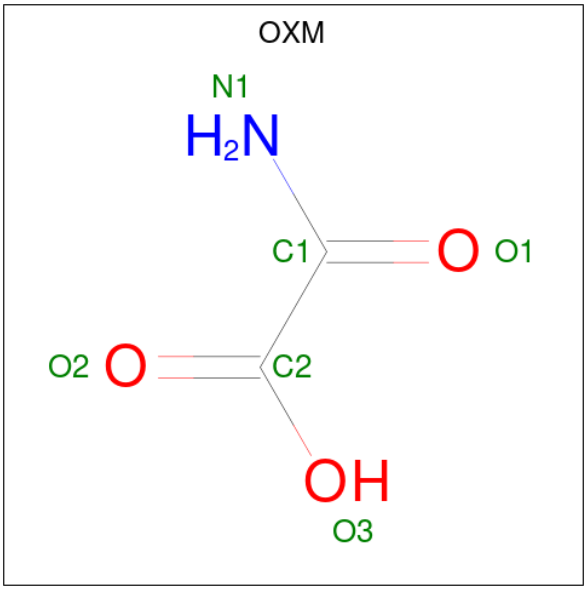
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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



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	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 O 76 76	0	0
5	B	77	Total O 77 77	0	0

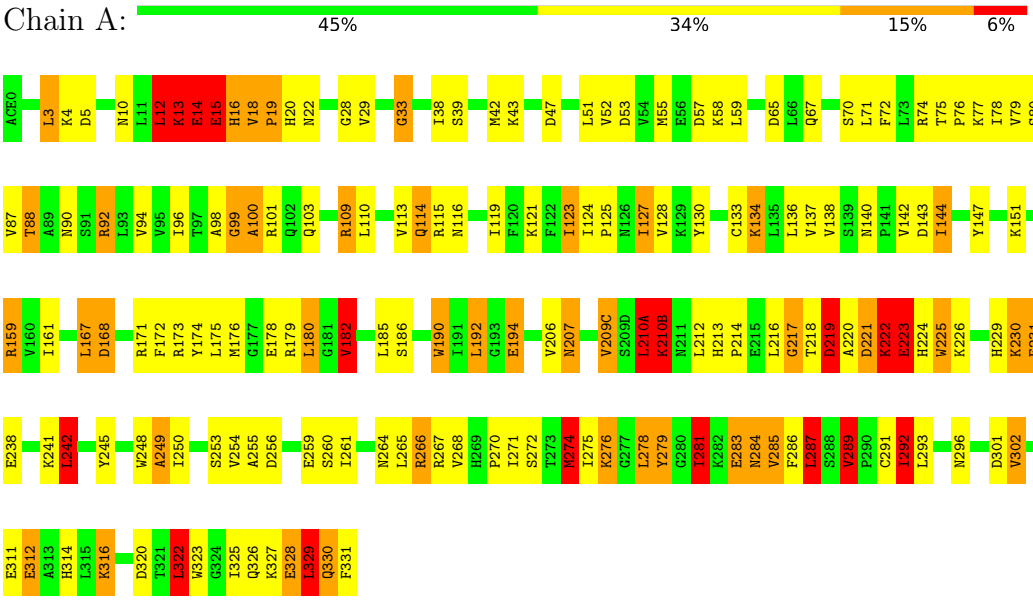
3 Residue-property plots (i)

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.

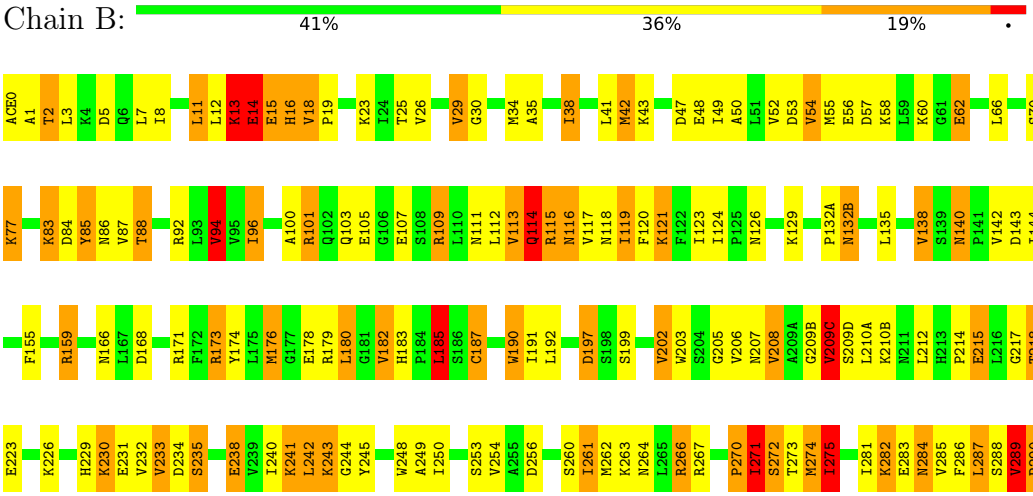
• Molecule 1: LACTATE DEHYDROGENASE

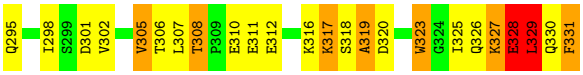
Chain A:



• Molecule 1: LACTATE DEHYDROGENASE

Chain B:




Q295
I298
S299
D301
V302
V305
T306
L307
T308
P309
E310
E311
E312
K316
K317
S318
A319
D320
W323
G324
I325
Q326
K327
E328
L329
Q330
F331

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 – 2.00	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: ACE, SO4, OXM, 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	1.07	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	8.46	1.34	1.25
1	A	74	ARG	CZ-NH2	5.22	1.39	1.33

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	ARG	NE-CZ-NH1	39.53	140.07	120.30
1	B	115	ARG	NE-CZ-NH2	39.13	139.87	120.30
1	A	159	ARG	NE-CZ-NH2	-34.14	103.23	120.30
1	A	179	ARG	NE-CZ-NH1	-28.09	106.25	120.30
1	B	221	ASP	C-N-CA	23.30	179.95	121.70
1	B	109	ARG	CD-NE-CZ	23.10	155.94	123.60
1	B	101	ARG	CD-NE-CZ	21.77	154.08	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	ARG	NE-CZ-NH1	-21.29	109.66	120.30
1	B	115	ARG	NE-CZ-NH1	-18.66	110.97	120.30
1	B	11	LEU	CA-CB-CG	17.20	154.87	115.30
1	B	101	ARG	CG-CD-NE	16.04	145.48	111.80
1	B	15	GLU	CA-CB-CG	15.71	147.97	113.40
1	A	312	GLU	CA-CB-CG	15.05	146.50	113.40
1	A	179	ARG	NE-CZ-NH2	14.70	127.65	120.30
1	A	266	ARG	NE-CZ-NH2	-14.59	113.01	120.30
1	B	197	ASP	CB-CG-OD2	-13.97	105.72	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	-13.33	106.30	118.30
1	A	301	ASP	CB-CG-OD1	13.21	130.19	118.30
1	B	12	LEU	CA-CB-CG	13.13	145.51	115.30
1	A	221	ASP	CB-CG-OD1	13.13	130.12	118.30
1	B	317	LYS	CA-CB-CG	12.82	141.60	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	-12.27	114.16	120.30
1	A	312	GLU	OE1-CD-OE2	-12.26	108.58	123.30
1	B	173	ARG	NE-CZ-NH1	12.23	126.41	120.30
1	B	179	ARG	CD-NE-CZ	12.07	140.50	123.60
1	A	55	MET	CG-SD-CE	-11.61	81.63	100.20
1	B	14	GLU	CA-C-O	11.54	144.33	120.10
1	B	266	ARG	CD-NE-CZ	11.43	139.59	123.60
1	B	119	ILE	CA-CB-CG2	11.28	133.45	110.90
1	A	272	SER	N-CA-CB	10.94	126.91	110.50
1	A	16	HIS	O-C-N	10.93	140.18	122.70
1	B	301	ASP	CB-CG-OD2	-10.91	108.48	118.30
1	B	234	ASP	CB-CG-OD2	-10.88	108.50	118.30
1	A	143	ASP	CB-CG-OD1	-10.85	108.54	118.30
1	B	179	ARG	NE-CZ-NH2	10.71	125.65	120.30
1	B	57	ASP	CB-CG-OD1	10.70	127.93	118.30
1	A	274	MET	CA-CB-CG	-10.62	95.25	113.30
1	A	42	MET	CG-SD-CE	-10.55	83.32	100.20
1	B	221	ASP	O-C-N	-10.47	105.94	122.70
1	A	219	ASP	CB-CG-OD1	-10.44	108.91	118.30
1	A	168	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	A	174	TYR	CB-CG-CD1	-10.39	114.77	121.00
1	A	267	ARG	NH1-CZ-NH2	10.38	130.81	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	ARG	NH1-CZ-NH2	10.26	130.68	119.40
1	B	105	GLU	CG-CD-OE1	10.24	138.78	118.30
1	B	266	ARG	NE-CZ-NH2	10.23	125.41	120.30
1	A	173	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	A	267	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	B	171	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	A	234	ASP	CB-CG-OD1	-10.07	109.24	118.30
1	B	2	THR	CA-CB-CG2	10.04	126.46	112.40
1	B	105	GLU	CG-CD-OE2	-9.99	98.31	118.30
1	A	115	ARG	NE-CZ-NH1	-9.77	115.41	120.30
1	A	84	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	B	301	ASP	CB-CG-OD1	9.64	126.98	118.30
1	A	157	LYS	CA-CB-CG	9.44	134.17	113.40
1	A	57	ASP	CB-CG-OD1	9.43	126.79	118.30
1	B	115	ARG	NH1-CZ-NH2	-9.41	109.05	119.40
1	B	289	VAL	CB-CA-C	9.37	129.20	111.40
1	B	243	LYS	CA-C-O	-9.25	100.68	120.10
1	A	267	ARG	CD-NE-CZ	-9.19	110.73	123.60
1	B	14	GLU	CA-C-N	-9.13	97.11	117.20
1	B	208	VAL	CA-CB-CG2	9.11	124.56	110.90
1	A	86	ASN	CB-CG-OD1	-9.10	103.40	121.60
1	A	283	GLU	OE1-CD-OE2	8.95	134.03	123.30
1	A	53	ASP	CB-CG-OD2	8.91	126.32	118.30
1	B	256	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	65	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	84	ASP	CB-CG-OD2	8.84	126.25	118.30
1	B	55	MET	CG-SD-CE	-8.83	86.07	100.20
1	B	57	ASP	CB-CG-OD2	-8.83	110.36	118.30
1	B	101	ARG	O-C-N	-8.80	108.62	122.70
1	B	101	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	A	217	GLY	C-N-CA	8.73	143.54	121.70
1	B	232	VAL	CA-CB-CG1	8.72	123.97	110.90
1	A	245	TYR	CB-CG-CD2	8.66	126.20	121.00
1	A	172	PHE	CB-CG-CD2	8.56	126.79	120.80
1	B	260	SER	N-CA-CB	8.54	123.30	110.50
1	A	77	LYS	O-C-N	8.51	136.31	122.70
1	B	166	ASN	CB-CG-ND2	8.43	136.93	116.70
1	A	328	GLU	CA-CB-CG	8.42	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	137.56	120.10
1	A	179	ARG	CD-NE-CZ	8.27	135.18	123.60
1	B	241	LYS	CA-CB-CG	8.26	131.56	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	CD-NE-CZ	8.19	135.06	123.60
1	A	87	VAL	CA-CB-CG2	8.14	123.11	110.90
1	A	13	LYS	CA-C-O	8.10	137.11	120.10
1	A	320	ASP	CA-CB-CG	8.10	131.21	113.40
1	B	16	HIS	CA-CB-CG	-8.09	99.84	113.60
1	B	159	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	B	289	VAL	N-CA-CB	-8.05	93.79	111.50
1	A	330	GLN	C-N-CA	7.97	141.63	121.70
1	B	179	ARG	NH1-CZ-NH2	-7.95	110.66	119.40
1	B	320	ASP	CB-CG-OD1	7.93	125.44	118.30
1	B	220	ALA	C-N-CA	7.93	141.52	121.70
1	A	130	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	B	221	ASP	CB-CG-OD1	7.92	125.43	118.30
1	B	219	ASP	CB-CA-C	7.92	126.24	110.40
1	B	85	TYR	N-CA-CB	7.92	124.85	110.60
1	B	221	ASP	N-CA-CB	-7.88	96.42	110.60
1	B	92	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	B	209(B)	GLY	CA-C-O	-7.82	106.53	120.60
1	B	43	LYS	C-N-CA	7.82	141.24	121.70
1	B	176	MET	CG-SD-CE	-7.80	87.72	100.20
1	A	307	LEU	CA-CB-CG	7.79	133.22	115.30
1	B	230	LYS	CD-CE-NZ	7.79	129.61	111.70
1	A	220	ALA	CA-C-O	-7.78	103.77	120.10
1	B	256	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	292	ILE	CB-CA-C	7.75	127.11	111.60
1	B	220	ALA	CB-CA-C	7.75	121.72	110.10
1	B	0	ACE	O-C-N	-7.65	110.46	122.70
1	B	203	TRP	N-CA-CB	7.65	124.37	110.60
1	B	48	GLU	CA-CB-CG	7.59	130.09	113.40
1	B	221	ASP	CA-CB-CG	7.50	129.91	113.40
1	B	92	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	274	MET	CG-SD-CE	-7.46	88.27	100.20
1	B	190	TRP	O-C-N	7.46	134.63	122.70
1	A	143	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	289	VAL	N-CA-CB	-7.44	95.14	111.50
1	B	272	SER	N-CA-CB	7.36	121.55	110.50
1	A	92	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	329	LEU	CA-CB-CG	7.34	132.17	115.30
1	B	180	LEU	N-CA-CB	-7.33	95.75	110.40
1	A	86	ASN	CA-CB-CG	7.32	129.50	113.40
1	B	152	ILE	CA-CB-CG1	7.30	124.88	111.00
1	A	289	VAL	CA-CB-CG1	7.29	121.84	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	THR	N-CA-CB	-7.26	96.51	110.30
1	A	276	LYS	CA-CB-CG	7.24	129.32	113.40
1	B	253	SER	N-CA-CB	7.23	121.34	110.50
1	B	70	SER	CA-CB-OG	-7.20	91.75	111.20
1	B	71	LEU	CB-CG-CD1	-7.17	98.81	111.00
1	A	47	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	77	LYS	N-CA-CB	7.14	123.45	110.60
1	B	38	ILE	CG1-CB-CG2	-7.12	95.74	111.40
1	A	223	GLU	C-N-CA	7.10	139.45	121.70
1	A	231	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	A	178	GLU	CB-CG-CD	7.09	133.35	114.20
1	A	266	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	B	92	ARG	NH1-CZ-NH2	-7.03	111.67	119.40
1	B	272	SER	O-C-N	7.03	133.95	122.70
1	A	292	ILE	CG1-CB-CG2	-7.03	95.94	111.40
1	A	207	ASN	O-C-N	7.02	133.93	122.70
1	B	205	GLY	CA-C-O	-7.02	107.97	120.60
1	B	327	LYS	O-C-N	-7.00	111.50	122.70
1	A	268	VAL	CA-CB-CG1	7.00	121.40	110.90
1	A	278	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	B	119	ILE	CB-CG1-CD1	-6.97	94.37	113.90
1	A	33	GLY	CA-C-O	-6.97	108.05	120.60
1	B	86	ASN	CB-CG-ND2	6.87	133.19	116.70
1	B	287	LEU	CB-CG-CD2	-6.84	99.37	111.00
1	A	210(A)	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	85	TYR	CB-CG-CD1	6.80	125.08	121.00
1	A	289	VAL	CB-CA-C	6.79	124.30	111.40
1	A	110	LEU	CB-CG-CD2	6.76	122.49	111.00
1	B	185	LEU	CA-CB-CG	6.74	130.79	115.30
1	A	253	SER	CA-C-N	6.72	131.99	117.20
1	B	323	TRP	CB-CG-CD1	6.68	135.69	127.00
1	A	185	LEU	CA-CB-CG	6.67	130.64	115.30
1	A	259	GLU	CG-CD-OE1	6.67	131.64	118.30
1	A	237	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	B	307	LEU	O-C-N	6.64	133.32	122.70
1	A	171	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	B	41	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	B	243	LYS	O-C-N	6.61	134.44	123.20
1	A	98	ALA	N-CA-CB	-6.61	100.85	110.10
1	A	223	GLU	OE1-CD-OE2	6.60	131.22	123.30
1	A	245	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	A	174	TYR	CB-CG-CD2	6.60	124.96	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	SER	CB-CA-C	-6.59	97.58	110.10
1	A	121	LYS	CA-CB-CG	6.58	127.87	113.40
1	B	320	ASP	OD1-CG-OD2	-6.58	110.81	123.30
1	A	312	GLU	CG-CD-OE1	6.57	131.45	118.30
1	B	221	ASP	CA-C-N	6.57	131.65	117.20
1	B	35	ALA	N-CA-CB	6.57	119.29	110.10
1	B	5	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	84	ASP	CA-C-N	6.55	131.61	117.20
1	A	256	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	287	LEU	CB-CA-C	6.51	122.56	110.20
1	B	48	GLU	N-CA-CB	6.50	122.30	110.60
1	A	281	ILE	CB-CA-C	6.49	124.58	111.60
1	B	116	ASN	CB-CA-C	6.49	123.37	110.40
1	A	237	TYR	O-C-N	6.48	133.06	122.70
1	A	278	LEU	CA-C-N	6.47	131.44	117.20
1	B	53	ASP	CB-CG-OD1	6.47	124.13	118.30
1	B	233	VAL	C-N-CA	6.47	137.87	121.70
1	A	58	LYS	CA-CB-CG	6.46	127.60	113.40
1	B	243	LYS	N-CA-CB	6.46	122.22	110.60
1	B	14	GLU	CA-CB-CG	6.45	127.60	113.40
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	222	LYS	N-CA-CB	6.44	122.19	110.60
1	A	222	LYS	N-CA-C	6.43	128.37	111.00
1	B	111	ASN	CA-C-O	-6.43	106.59	120.10
1	A	249	ALA	N-CA-CB	-6.42	101.12	110.10
1	B	119	ILE	CG1-CB-CG2	-6.41	97.31	111.40
1	A	110	LEU	CB-CA-C	6.40	122.36	110.20
1	B	66	LEU	CB-CG-CD1	-6.37	100.16	111.00
1	B	323	TRP	CD1-NE1-CE2	-6.37	103.27	109.00
1	B	266	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	B	14	GLU	C-N-CA	6.34	137.55	121.70
1	A	134	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	A	70	SER	CA-CB-OG	-6.32	94.13	111.20
1	A	155	PHE	CB-CG-CD1	-6.32	116.38	120.80
1	B	155	PHE	O-C-N	6.31	133.09	121.10
1	B	319	ALA	N-CA-CB	6.30	118.92	110.10
1	A	16	HIS	CA-C-N	-6.30	103.34	117.20
1	A	278	LEU	CA-C-O	-6.29	106.89	120.10
1	A	13	LYS	C-N-CA	6.28	137.40	121.70
1	A	29	VAL	O-C-N	-6.28	112.53	123.20
1	B	327	LYS	C-N-CA	6.28	137.39	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	209(C)	VAL	CA-C-O	6.27	133.26	120.10
1	B	284	ASN	CA-CB-CG	6.26	127.17	113.40
1	B	13	LYS	CA-C-O	6.24	133.20	120.10
1	A	225	TRP	O-C-N	6.24	132.68	122.70
1	A	190	TRP	CD1-CG-CD2	-6.23	101.32	106.30
1	B	178	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	B	290	PRO	CB-CA-C	6.20	127.51	112.00
1	A	292	ILE	CB-CA-C	6.20	124.00	111.60
1	A	103	GLN	CB-CG-CD	6.20	127.72	111.60
1	A	302	VAL	CA-C-N	6.19	130.82	117.20
1	B	174	TYR	O-C-N	-6.19	112.80	122.70
1	A	231	GLU	CA-CB-CG	6.18	126.99	113.40
1	B	26	VAL	CA-CB-CG2	6.17	120.15	110.90
1	A	12	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	190	TRP	NE1-CE2-CZ2	-6.15	123.63	130.40
1	A	219	ASP	OD1-CG-OD2	6.14	134.97	123.30
1	B	242	LEU	CA-C-O	-6.14	107.21	120.10
1	B	111	ASN	CA-C-N	6.13	130.69	117.20
1	A	238	GLU	OE1-CD-OE2	6.13	130.65	123.30
1	A	219	ASP	CA-CB-CG	6.13	126.88	113.40
1	A	222	LYS	C-N-CA	6.13	137.01	121.70
1	A	79	VAL	CA-CB-CG1	6.12	120.08	110.90
1	B	222	LYS	CB-CA-C	-6.12	98.16	110.40
1	B	222	LYS	N-CA-C	6.12	127.52	111.00
1	B	112	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	B	328	GLU	CA-CB-CG	6.11	126.83	113.40
1	A	176	MET	CG-SD-CE	-6.10	90.45	100.20
1	A	179	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	A	307	LEU	O-C-N	6.08	132.43	122.70
1	A	267	ARG	CB-CG-CD	-6.07	95.82	111.60
1	B	249	ALA	O-C-N	6.06	132.40	122.70
1	B	13	LYS	CA-CB-CG	6.06	126.73	113.40
1	A	67	GLN	C-N-CA	6.04	136.81	121.70
1	A	192	LEU	O-C-N	-6.03	112.94	123.20
1	A	65	ASP	CA-C-O	-6.01	107.47	120.10
1	A	16	HIS	CB-CA-C	6.01	122.42	110.40
1	B	176	MET	C-N-CA	6.00	134.90	122.30
1	A	100	ALA	O-C-N	5.99	132.29	122.70
1	B	254	VAL	CA-CB-CG2	-5.99	101.92	110.90
1	B	235	SER	CB-CA-C	5.98	121.47	110.10
1	A	144	ILE	CA-CB-CG1	-5.98	99.64	111.00
1	A	219	ASP	N-CA-C	5.97	127.13	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	LEU	O-C-N	5.97	132.25	122.70
1	A	5	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	B	118	ASN	CA-CB-CG	-5.97	100.27	113.40
1	B	62	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	A	222	LYS	N-CA-CB	-5.96	99.87	110.60
1	A	310	GLU	CB-CG-CD	5.96	130.29	114.20
1	A	190	TRP	CD1-NE1-CE2	-5.94	103.65	109.00
1	A	113	VAL	CB-CA-C	5.93	122.66	111.40
1	B	318	SER	O-C-N	-5.92	113.23	122.70
1	B	329	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	220	ALA	O-C-N	5.90	132.14	122.70
1	A	101	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	78	ILE	O-C-N	5.89	132.12	122.70
1	B	0	ACE	C-N-CA	5.88	136.41	121.70
1	B	312	GLU	CG-CD-OE2	-5.88	106.53	118.30
1	A	92	ARG	CB-CG-CD	5.88	126.89	111.60
1	B	320	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	202	VAL	CG1-CB-CG2	-5.88	101.50	110.90
1	B	328	GLU	CB-CA-C	-5.87	98.67	110.40
1	B	262	MET	CG-SD-CE	-5.87	90.81	100.20
1	A	190	TRP	CB-CG-CD2	5.86	134.22	126.60
1	A	309	PRO	CA-C-N	5.86	130.09	117.20
1	A	242	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	174	TYR	CA-CB-CG	-5.85	102.28	113.40
1	A	79	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	A	178	GLU	CG-CD-OE1	5.84	129.99	118.30
1	A	210(B)	LYS	CA-C-N	5.84	130.05	117.20
1	B	210(A)	LEU	CB-CA-C	5.83	121.28	110.20
1	A	75	THR	CA-CB-CG2	-5.83	104.24	112.40
1	A	328	GLU	CG-CD-OE1	5.80	129.90	118.30
1	A	38	ILE	CA-CB-CG2	5.80	122.50	110.90
1	A	147	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	43	LYS	CB-CG-CD	-5.78	96.57	111.60
1	A	322	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	190	TRP	CB-CG-CD1	-5.76	119.51	127.00
1	A	302	VAL	O-C-N	-5.75	113.50	122.70
1	A	13	LYS	CA-CB-CG	5.74	126.02	113.40
1	B	50	ALA	N-CA-CB	5.74	118.13	110.10
1	B	86	ASN	OD1-CG-ND2	-5.73	108.71	121.90
1	B	275	ILE	CA-CB-CG1	-5.73	100.11	111.00
1	B	249	ALA	CA-C-O	-5.72	108.09	120.10
1	A	209(C)	VAL	CA-CB-CG1	5.72	119.48	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	293	LEU	CA-C-N	5.70	127.59	116.20
1	B	138	VAL	CG1-CB-CG2	-5.69	101.79	110.90
1	A	65	ASP	OD1-CG-OD2	5.68	134.10	123.30
1	A	281	ILE	N-CA-C	-5.67	95.68	111.00
1	A	267	ARG	CG-CD-NE	-5.67	99.90	111.80
1	B	292	ILE	CA-CB-CG1	-5.67	100.24	111.00
1	B	241	LYS	CG-CD-CE	5.66	128.88	111.90
1	A	261	ILE	O-C-N	-5.65	113.66	122.70
1	A	57	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	221	ASP	CA-CB-CG	5.64	125.82	113.40
1	A	173	ARG	NH1-CZ-NH2	5.63	125.59	119.40
1	A	255	ALA	C-N-CA	5.62	135.76	121.70
1	B	223	GLU	C-N-CA	5.62	135.76	121.70
1	B	26	VAL	O-C-N	5.62	131.69	122.70
1	B	2	THR	CA-CB-OG1	-5.61	97.21	109.00
1	A	52	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	A	59	LEU	O-C-N	5.61	131.67	122.70
1	B	35	ALA	O-C-N	5.61	131.67	122.70
1	A	186	SER	CA-C-O	-5.59	108.36	120.10
1	A	109	ARG	CG-CD-NE	5.59	123.53	111.80
1	B	107	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	A	283	GLU	O-C-N	5.56	131.60	122.70
1	B	270	PRO	CA-C-O	-5.56	106.85	120.20
1	A	267	ARG	CA-CB-CG	-5.55	101.18	113.40
1	B	287	LEU	CA-C-O	-5.54	108.46	120.10
1	B	182	VAL	CG1-CB-CG2	-5.54	102.04	110.90
1	B	261	ILE	O-C-N	-5.54	113.84	122.70
1	B	166	ASN	OD1-CG-ND2	-5.53	109.18	121.90
1	A	114	GLN	N-CA-CB	5.53	120.55	110.60
1	B	274	MET	N-CA-CB	-5.52	100.66	110.60
1	B	70	SER	CB-CA-C	-5.52	99.61	110.10
1	A	311	GLU	CG-CD-OE2	-5.51	107.27	118.30
1	B	126	ASN	CB-CG-OD1	-5.51	110.59	121.60
1	A	86	ASN	CB-CG-ND2	5.50	129.91	116.70
1	B	114	GLN	CB-CG-CD	5.50	125.91	111.60
1	B	263	LYS	CA-C-O	-5.50	108.55	120.10
1	A	192	LEU	N-CA-CB	-5.49	99.42	110.40
1	A	3	LEU	CB-CA-C	5.48	120.62	110.20
1	B	329	LEU	CB-CA-C	5.47	120.59	110.20
1	B	205	GLY	CA-C-N	5.46	129.22	117.20
1	A	159	ARG	CA-CB-CG	5.45	125.40	113.40
1	B	302	VAL	CA-C-N	5.45	129.19	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	GLU	CB-CG-CD	5.45	128.90	114.20
1	B	42	MET	CA-CB-CG	-5.44	104.04	113.30
1	A	92	ARG	CD-NE-CZ	-5.44	115.99	123.60
1	B	29	VAL	CG1-CB-CG2	-5.43	102.22	110.90
1	B	305	VAL	CB-CA-C	5.42	121.70	111.40
1	A	53	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	74	ARG	CG-CD-NE	5.41	123.17	111.80
1	A	171	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	B	74	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	A	137	VAL	O-C-N	5.41	131.35	122.70
1	A	14	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	A	167	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	B	323	TRP	CB-CG-CD2	-5.39	119.59	126.60
1	A	210(B)	LYS	O-C-N	-5.38	114.09	122.70
1	B	54	VAL	CB-CA-C	-5.38	101.17	111.40
1	B	254	VAL	CG1-CB-CG2	5.37	119.50	110.90
1	B	94	VAL	CA-CB-CG1	5.37	118.95	110.90
1	B	250	ILE	CA-C-N	5.36	126.93	116.20
1	B	190	TRP	CA-C-N	-5.36	105.41	117.20
1	A	278	LEU	CB-CG-CD1	5.35	120.10	111.00
1	B	140	ASN	CB-CG-OD1	5.35	132.30	121.60
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	96	ILE	CA-C-N	-5.34	105.45	117.20
1	A	207	ASN	N-CA-CB	-5.33	101.01	110.60
1	A	285	VAL	CA-CB-CG1	5.33	118.89	110.90
1	B	187	CYS	N-CA-CB	5.32	120.18	110.60
1	B	77	LYS	CG-CD-CE	5.32	127.87	111.90
1	A	109	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	B	256	ASP	CA-C-O	5.30	131.24	120.10
1	B	271	ILE	CA-C-O	-5.30	108.97	120.10
1	A	172	PHE	CG-CD2-CE2	5.30	126.63	120.80
1	A	99	GLY	CA-C-N	-5.29	105.55	117.20
1	B	121	LYS	CA-CB-CG	5.29	125.04	113.40
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	A	18	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	A	329	LEU	C-N-CA	5.26	134.84	121.70
1	B	238	GLU	CA-C-N	5.25	128.76	117.20
1	A	182	VAL	CA-CB-CG1	-5.25	103.02	110.90
1	B	103	GLN	N-CA-C	-5.25	96.84	111.00
1	B	323	TRP	CG-CD2-CE3	-5.24	129.19	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	TRP	CB-CG-CD2	5.24	133.41	126.60
1	A	296	ASN	CA-C-O	-5.24	109.11	120.10
1	A	123	ILE	O-C-N	5.23	131.07	122.70
1	A	260	SER	N-CA-CB	5.23	118.34	110.50
1	A	85	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	222	LYS	O-C-N	-5.22	114.35	122.70
1	B	263	LYS	CD-CE-NZ	-5.22	99.69	111.70
1	B	209(C)	VAL	CB-CA-C	5.21	121.29	111.40
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	5.19	122.97	118.30
1	A	59	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	A	264	ASN	CB-CG-OD1	5.18	131.95	121.60
1	A	259	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	B	12	LEU	CB-CA-C	-5.17	100.38	110.20
1	A	86	ASN	N-CA-CB	-5.17	101.30	110.60
1	B	143	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	180	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	A	20	HIS	O-C-N	5.16	130.95	122.70
1	A	72	PHE	CZ-CE2-CD2	-5.16	113.91	120.10
1	A	13	LYS	CA-C-N	-5.15	105.86	117.20
1	B	144	ILE	CA-C-N	5.15	128.54	117.20
1	B	208	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	A	279	TYR	CG-CD1-CE1	5.15	125.42	121.30
1	B	5	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	261	ILE	CA-C-N	5.14	128.50	117.20
1	A	279	TYR	CB-CG-CD2	5.14	124.08	121.00
1	A	194	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	A	291	CYS	N-CA-CB	5.13	119.83	110.60
1	B	168	ASP	O-C-N	5.13	130.91	122.70
1	A	182	VAL	CA-CB-CG2	5.12	118.58	110.90
1	A	221	ASP	CA-C-O	5.12	130.85	120.10
1	B	248	TRP	CD1-NE1-CE2	-5.12	104.39	109.00
1	B	263	LYS	CA-CB-CG	-5.11	102.16	113.40
1	A	289	VAL	CA-C-O	-5.10	109.40	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	A	67	GLN	O-C-N	-5.08	114.58	122.70
1	A	12	LEU	O-C-N	5.07	130.81	122.70
1	B	232	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	A	320	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	58	LYS	C-N-CA	5.06	134.34	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	242	LEU	O-C-N	5.06	130.79	122.70
1	B	238	GLU	CA-C-O	-5.05	109.48	120.10
1	B	48	GLU	O-C-N	5.05	130.78	122.70
1	B	114	GLN	CB-CA-C	5.04	120.49	110.40
1	A	283	GLU	CA-C-N	-5.04	106.11	117.20
1	A	15	GLU	C-N-CA	-5.04	109.10	121.70
1	A	18	VAL	CA-CB-CG1	5.03	118.45	110.90
1	B	306	THR	C-N-CA	5.03	134.28	121.70
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	171	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	B	191	ILE	N-CA-CB	5.02	122.34	110.80
1	A	16	HIS	N-CA-C	-5.01	97.46	111.00
1	A	327	LYS	CA-CB-CG	5.01	124.42	113.40
1	B	87	VAL	C-N-CA	5.01	134.22	121.70
1	B	96	ILE	CA-C-O	5.01	130.62	120.10
1	A	90	ASN	CA-C-O	5.00	130.60	120.10

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 (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	93	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	2	0	0
5	A	76	0	0	6	0
5	B	77	0	0	11	0
All	All	5399	0	5338	180	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 (180) 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	1.14
1:A:221:ASP:O	1:A:222:LYS:HB2	1.48	1.09
1:B:217:GLY:O	1:B:219:ASP:N	1.93	1.01
1:A:100:ALA:H	1:A:116:ASN:HD21	1.04	0.95
1:A:18:VAL:HG23	1:A:19:PRO:HD2	1.53	0.90
1:A:43:LYS:HE3	5:A:474:HOH:O	1.69	0.90
1:B:100:ALA:H	1:B:116:ASN:HD21	1.20	0.90
5:A:479:HOH:O	1:B:2:THR:HG22	1.73	0.86
1:B:13:LYS:CG	1:B:14:GLU:H	1.83	0.85
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	0.84
1:A:85:TYR:O	1:A:88:THR:HB	1.78	0.82
1:B:114:GLN:HG3	1:B:330:GLN:HE22	1.45	0.81
1:B:132(A):PRO:O	1:B:159:ARG:NH1	2.13	0.80
1:B:217:GLY:C	1:B:219:ASP:H	1.85	0.78
1:A:4:LYS:HE3	5:A:439:HOH:O	1.87	0.74
1:A:10:ASN:ND2	1:A:12:LEU:O	2.20	0.73
1:B:77:LYS:HE3	5:B:456:HOH:O	1.88	0.72
1:B:266:ARG:HB3	1:B:292:ILE:HD11	1.71	0.72
1:A:274:MET:HG3	1:A:286:PHE:CE2	2.26	0.71
1:A:221:ASP:O	1:A:222:LYS:CB	2.32	0.70
1:B:290:PRO:HG2	1:B:305:VAL:HG11	1.74	0.70
1:A:222:LYS:HG2	1:A:223:GLU:H	1.55	0.70
1:B:238:GLU:O	1:B:242:LEU:HD12	1.91	0.69
1:B:114:GLN:HG3	1:B:330:GLN:NE2	2.07	0.68
1:B:123:ILE:HG13	1:B:124:ILE:N	2.09	0.68
1:A:14:GLU:C	1:A:15:GLU:O	2.28	0.68
1:A:266:ARG:HB3	1:A:292:ILE:HD13	1.77	0.67
1:B:329:LEU:HA	1:B:331:PHE:CE1	2.29	0.67
1:B:132(B):ASN:HA	1:B:159:ARG:NH1	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD13	1:A:231:GLU:HG3	1.76	0.67
1:A:289:VAL:HG13	1:A:302:VAL:HG13	1.77	0.66
1:A:242:LEU:HD21	1:B:60:LYS:HD3	1.76	0.66
1:B:243:LYS:HE2	1:B:245:TYR:O	1.96	0.65
1:B:13:LYS:HG3	1:B:14:GLU:H	1.61	0.65
1:A:230:LYS:HE3	5:A:421:HOH:O	1.97	0.65
1:A:210(A):LEU:HD11	1:B:7:LEU:HD22	1.77	0.65
1:A:217:GLY:H	1:A:222:LYS:HZ2	1.44	0.65
1:B:88:THR:CG2	5:B:453:HOH:O	2.45	0.64
1:A:217:GLY:H	1:A:222:LYS:NZ	1.94	0.64
1:A:100:ALA:N	1:A:116:ASN:HD21	1.87	0.63
1:B:261:ILE:HG13	1:B:293:LEU:HD13	1.81	0.63
1:B:275:ILE:CD1	1:B:281:ILE:HG13	2.30	0.62
1:A:138:VAL:O	3:A:401:NAD:H2N	2.00	0.62
1:B:100:ALA:N	1:B:116:ASN:HD21	1.94	0.61
1:B:176:MET:CE	1:B:206:VAL:HG11	2.30	0.61
1:A:281:ILE:C	1:A:281:ILE:HD13	2.21	0.60
1:A:210(A):LEU:HG	1:B:3:LEU:HD21	1.82	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	0.60
1:A:275:ILE:HD12	1:A:281:ILE:HG21	1.83	0.60
1:A:39:SER:HA	1:B:42:MET:HE3	1.83	0.60
1:B:199:SER:OG	1:B:229:HIS:HE1	1.85	0.59
1:A:161:ILE:CG2	1:A:271:ILE:HD12	2.30	0.59
1:A:94:VAL:HG21	1:A:127:ILE:HD13	1.84	0.59
1:B:176:MET:HE1	1:B:206:VAL:HG11	1.84	0.58
1:A:316:LYS:HE3	1:A:316:LYS:HA	1.85	0.58
1:A:190:TRP:CZ3	1:A:270:PRO:HD3	2.37	0.58
1:A:289:VAL:HG13	1:A:302:VAL:CG1	2.34	0.58
1:A:222:LYS:CG	1:A:223:GLU:H	2.10	0.58
1:B:274:MET:CG	1:B:286:PHE:CE2	2.87	0.58
1:B:117:VAL:HG22	1:B:148:VAL:HG21	1.86	0.57
1:B:58:LYS:NZ	5:B:472:HOH:O	2.18	0.57
1:A:127:ILE:HD11	1:A:133:CYS:SG	2.44	0.57
1:A:14:GLU:O	1:A:15:GLU:O	2.22	0.56
1:B:190:TRP:HB3	1:B:192:LEU:HD13	1.86	0.56
1:B:16:HIS:O	1:B:16:HIS:CG	2.55	0.56
1:A:13:LYS:O	1:A:15:GLU:N	2.39	0.56
1:A:289:VAL:CG1	1:A:302:VAL:HG13	2.35	0.55
1:A:4:LYS:CG	5:B:406:HOH:O	2.24	0.55
1:B:182:VAL:HG23	1:B:187:CYS:SG	2.46	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:HD11	1:B:135:LEU:HD22	1.88	0.55
1:B:182:VAL:CG2	1:B:187:CYS:SG	2.95	0.54
1:A:22:ASN:HD22	1:A:92:ARG:HH21	1.54	0.54
1:B:16:HIS:O	1:B:16:HIS:ND1	2.41	0.54
1:B:88:THR:HG22	5:B:453:HOH:O	2.07	0.54
1:A:39:SER:HA	1:B:42:MET:CE	2.38	0.53
1:B:271:ILE:O	1:B:288:SER:HA	2.07	0.53
1:B:274:MET:HG3	1:B:286:PHE:CE2	2.43	0.53
1:B:7:LEU:HG	1:B:8:ILE:HG13	1.91	0.53
1:B:308:THR:HG22	1:B:311:GLU:HG3	1.90	0.53
1:A:4:LYS:HD3	5:B:406:HOH:O	2.09	0.53
1:A:292:ILE:C	1:A:292:ILE:HD12	2.29	0.53
1:B:328:GLU:O	1:B:328:GLU:HG2	2.08	0.53
1:B:29:VAL:HG12	1:B:62:GLU:HG3	1.91	0.53
1:B:77:LYS:CE	5:B:456:HOH:O	2.52	0.52
1:A:194:GLU:HG3	1:A:322:LEU:CD1	2.40	0.52
1:B:56:GLU:OE1	1:B:83:LYS:HE2	2.09	0.52
1:B:120:PHE:HA	1:B:123:ILE:HG12	1.92	0.52
1:B:285:VAL:HG21	1:B:319:ALA:HB1	1.92	0.52
1:A:4:LYS:CD	5:B:406:HOH:O	2.53	0.52
1:B:275:ILE:HG12	1:B:287:LEU:HG	1.90	0.52
1:B:115:ARG:HD3	5:B:420:HOH:O	2.10	0.51
1:A:222:LYS:HD2	1:A:225:TRP:H	1.75	0.51
1:B:266:ARG:HB3	1:B:292:ILE:CD1	2.39	0.51
1:A:180:LEU:HB3	1:A:182:VAL:HG23	1.93	0.51
1:B:183:HIS:ND1	1:B:185:LEU:HB2	2.26	0.51
1:A:309:PRO:O	1:A:310:GLU:C	2.46	0.51
1:B:282:LYS:NZ	1:B:283:GLU:OE1	2.37	0.51
1:A:51:LEU:O	1:A:80:SER:HA	2.11	0.50
1:B:215:GLU:O	1:B:219:ASP:HB2	2.11	0.50
1:A:127:ILE:HG13	1:A:128:VAL:N	2.27	0.50
1:A:287:LEU:C	1:A:287:LEU:HD12	2.31	0.50
1:B:231:GLU:O	1:B:235:SER:HB3	2.12	0.50
1:B:18:VAL:HG23	1:B:19:PRO:HD2	1.92	0.49
1:A:22:ASN:ND2	1:A:92:ARG:HH21	2.10	0.49
1:A:316:LYS:HA	1:A:316:LYS:CE	2.42	0.49
1:B:29:VAL:CG1	1:B:62:GLU:HG3	2.43	0.49
1:A:85:TYR:CE2	1:A:127:ILE:HG22	2.48	0.49
1:A:15:GLU:O	1:A:16:HIS:CD2	2.65	0.49
1:B:192:LEU:HD22	1:B:202:VAL:HG21	1.93	0.49
1:A:144:ILE:HD13	1:A:325:ILE:HG21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210(B):LYS:NZ	1:A:214:PRO:O	2.42	0.48
1:B:328:GLU:O	1:B:330:GLN:N	2.46	0.48
1:A:124:ILE:HB	1:A:125:PRO:HD3	1.96	0.48
1:A:14:GLU:O	1:A:16:HIS:HD2	1.97	0.48
1:A:167:LEU:HD11	1:A:249:ALA:HB1	1.96	0.48
1:A:99:GLY:HA2	1:A:119:ILE:HD13	1.95	0.48
1:B:274:MET:HG2	1:B:286:PHE:CE2	2.49	0.47
1:A:71:LEU:HD12	1:B:185:LEU:HD13	1.96	0.47
1:A:210(A):LEU:CD1	1:B:7:LEU:HD22	2.44	0.47
1:A:217:GLY:N	1:A:222:LYS:NZ	2.62	0.47
1:B:16:HIS:CD2	1:B:16:HIS:C	2.87	0.46
1:B:285:VAL:HG12	1:B:326:GLN:NE2	2.30	0.46
1:A:217:GLY:O	1:A:219:ASP:OD2	2.33	0.46
1:A:123:ILE:O	1:A:127:ILE:HG23	2.15	0.46
1:A:206:VAL:HG12	1:A:210(A):LEU:HD22	1.97	0.46
1:A:159:ARG:HH21	1:A:159:ARG:HG3	1.81	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:183:HIS:CE1	1:B:185:LEU:HD22	2.51	0.46
1:A:28:GLY:O	1:A:33:GLY:HA3	2.16	0.46
1:A:194:GLU:HG3	1:A:322:LEU:HD13	1.97	0.46
1:A:285:VAL:HG22	1:A:323:TRP:HB2	1.98	0.46
1:B:109:ARG:HD3	1:B:140:ASN:OD1	2.16	0.45
1:B:190:TRP:HE3	1:B:270:PRO:HB3	1.82	0.45
1:B:240:ILE:O	1:B:244:GLY:N	2.49	0.44
1:B:173:ARG:NE	1:B:187:CYS:O	2.49	0.44
1:B:308:THR:HG23	1:B:310:GLU:OE1	2.18	0.44
1:B:208:VAL:O	1:B:209(C):VAL:HG13	2.17	0.44
1:A:234:ASP:HA	1:A:237:TYR:HD1	1.83	0.44
1:B:19:PRO:HB2	1:B:23:LYS:HB2	2.00	0.44
1:A:216:LEU:HA	1:A:222:LYS:HD3	2.00	0.44
1:A:307:LEU:HD13	1:A:312:GLU:HA	1.99	0.44
1:A:19:PRO:O	1:A:19:PRO:HG2	2.17	0.44
1:B:215:GLU:HG2	1:B:222:LYS:HZ2	1.81	0.44
1:B:243:LYS:HE3	1:B:245:TYR:CE2	2.52	0.44
1:A:283:GLU:HB3	1:A:284:ASN:H	1.60	0.43
1:B:289:VAL:HA	1:B:290:PRO:HD3	1.71	0.43
1:A:109:ARG:HG3	5:A:408:HOH:O	2.17	0.43
1:A:222:LYS:HB3	1:A:224:HIS:H	1.84	0.43
1:A:250:ILE:O	1:A:254:VAL:HG23	2.19	0.43
1:B:25:THR:HB	1:B:94:VAL:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLY:HA3	3:B:401:NAD:O5B	2.19	0.43
1:B:140:ASN:HA	1:B:142:VAL:N	2.34	0.43
1:A:326:GLN:HA	1:A:329:LEU:HD22	1.99	0.43
1:A:13:LYS:CB	1:A:14:GLU:HG3	2.49	0.43
1:A:276:LYS:HB2	1:A:283:GLU:O	2.18	0.43
1:B:273:THR:HB	1:B:298:ILE:HD12	2.00	0.42
1:A:190:TRP:HB3	1:A:192:LEU:HD13	2.01	0.42
1:A:279:TYR:N	1:A:281:ILE:HG22	2.33	0.42
1:B:115:ARG:CD	5:B:420:HOH:O	2.65	0.42
1:B:113:VAL:O	1:B:117:VAL:HG23	2.18	0.42
1:A:140:ASN:HA	1:A:142:VAL:N	2.34	0.42
1:B:210(B):LYS:NZ	1:B:214:PRO:O	2.52	0.42
1:B:85:TYR:O	1:B:88:THR:HB	2.20	0.41
1:A:229:HIS:HD2	5:A:419:HOH:O	2.03	0.41
1:A:316:LYS:CE	1:A:316:LYS:CA	2.98	0.41
1:B:138:VAL:O	3:B:401:NAD:H2N	2.21	0.41
1:B:190:TRP:HB3	1:B:192:LEU:CD1	2.51	0.41
1:B:275:ILE:HD12	1:B:281:ILE:HG21	2.02	0.41
1:B:282:LYS:H	1:B:282:LYS:HG3	1.49	0.41
1:A:213:HIS:HD2	1:A:216:LEU:HB2	1.86	0.41
1:B:264:ASN:HB2	1:B:295:GLN:HB3	2.02	0.41
1:B:282:LYS:HD2	1:B:283:GLU:OE1	2.21	0.40
1:A:85:TYR:HE2	1:A:127:ILE:HG22	1.86	0.40
1:B:29:VAL:HG13	1:B:34:MET:SD	2.61	0.40
1:B:197:ASP:HA	1:B:233:VAL:HG13	2.04	0.40
1:A:194:GLU:HG3	1:A:322:LEU:HD11	2.04	0.40
1:A:13:LYS:HB2	1:A:14:GLU:HG3	2.02	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 (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%)	301 (91%)	23 (7%)	6 (2%)	8 3
1	B	330/332 (99%)	304 (92%)	19 (6%)	7 (2%)	7 2
All	All	660/664 (99%)	605 (92%)	42 (6%)	13 (2%)	7 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 (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%)	246 (86%)	39 (14%)	3 2
1	B	285/285 (100%)	244 (86%)	41 (14%)	3 1
All	All	570/570 (100%)	490 (86%)	80 (14%)	3 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
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

Continued on next page...

Continued from previous page...

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	16	HIS
1	A	22	ASN
1	A	102	GLN
1	A	116	ASN
1	A	207	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 monosaccharides 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	B	401	-	42,48,48	1.93	6 (14%)	50,73,73	2.73	19 (38%)
2	SO4	B	403	-	4,4,4	0.87	0	6,6,6	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OXM	B	402	-	5,5,5	7.92	4 (80%)	4,6,6	8.43	2 (50%)
4	OXM	A	402	-	5,5,5	8.24	4 (80%)	4,6,6	9.68	3 (75%)
2	SO4	A	403	-	4,4,4	0.85	0	6,6,6	1.29	1 (16%)
3	NAD	A	401	-	42,48,48	3.01	6 (14%)	50,73,73	4.54	22 (44%)

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
4	OXM	A	402	-	-	2/3/4/4	-
3	NAD	B	401	-	-	4/26/62/62	0/5/5/5
4	OXM	B	402	-	-	0/3/4/4	-
3	NAD	A	401	-	-	4/26/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C3N-C7N	14.52	1.72	1.50
4	B	402	OXM	C1-C2	-12.37	1.39	1.55
4	A	402	OXM	C1-C2	-12.36	1.39	1.55
4	A	402	OXM	C1-N1	11.49	1.64	1.33
4	B	402	OXM	C1-N1	10.64	1.61	1.33
3	B	401	NAD	O7N-C7N	-8.32	1.08	1.24
3	A	401	NAD	C2N-N1N	7.34	1.43	1.35
3	A	401	NAD	C6N-N1N	7.08	1.52	1.35
4	A	402	OXM	O1-C1	6.57	1.40	1.24
4	B	402	OXM	O1-C1	5.16	1.36	1.24
3	B	401	NAD	C3N-C7N	5.15	1.58	1.50
4	B	402	OXM	O2-C2	4.55	1.34	1.22
3	B	401	NAD	C5N-C4N	-3.63	1.31	1.38
3	B	401	NAD	C6N-N1N	3.50	1.44	1.35
4	A	402	OXM	O2-C2	3.36	1.31	1.22
3	A	401	NAD	C2B-C1B	-3.34	1.48	1.53
3	A	401	NAD	C5N-C4N	-3.27	1.32	1.38
3	A	401	NAD	C2N-C3N	-2.68	1.34	1.39
3	B	401	NAD	C7N-N7N	-2.51	1.28	1.33
3	B	401	NAD	PA-O1A	-2.02	1.43	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	NAD	O7N-C7N-N7N	16.71	146.31	122.58
4	B	402	OXM	O3-C2-C1	12.47	142.67	113.84
3	A	401	NAD	C5A-C6A-N6A	12.40	139.19	120.35
3	A	401	NAD	O7N-C7N-C3N	-11.94	105.34	119.63
4	A	402	OXM	O2-C2-C1	-11.32	96.86	122.06
4	A	402	OXM	O1-C1-N1	-11.28	96.50	122.88
4	B	402	OXM	O2-C2-C1	-11.22	97.09	122.06
4	A	402	OXM	O3-C2-O2	10.93	148.62	123.61
3	A	401	NAD	C2N-C3N-C4N	8.55	127.95	118.26
3	A	401	NAD	C3N-C7N-N7N	-7.85	108.33	117.75
3	A	401	NAD	N6A-C6A-N1A	-7.62	102.77	118.57
3	A	401	NAD	C3N-C2N-N1N	-7.36	113.23	120.43
3	B	401	NAD	O7N-C7N-N7N	7.06	132.61	122.58
3	A	401	NAD	C5N-C6N-N1N	-6.32	111.33	120.40
3	B	401	NAD	O4D-C1D-C2D	-6.01	98.14	106.93
3	B	401	NAD	C6N-N1N-C2N	-5.35	117.10	121.97
3	B	401	NAD	C3N-C7N-N7N	-5.29	111.40	117.75
3	B	401	NAD	O4B-C1B-C2B	-5.01	99.60	106.93
3	B	401	NAD	C2N-C3N-C4N	4.84	123.75	118.26
3	B	401	NAD	C5A-C6A-N6A	4.72	127.52	120.35
3	B	401	NAD	C5N-C4N-C3N	-4.44	115.09	120.34
3	A	401	NAD	C2N-N1N-C1D	-4.31	109.54	119.14
3	A	401	NAD	C1B-N9A-C4A	-4.17	119.32	126.64
3	B	401	NAD	O7N-C7N-C3N	-3.99	114.86	119.63
3	A	401	NAD	O2D-C2D-C3D	3.67	123.68	111.82
3	A	401	NAD	C4A-C5A-N7A	-3.53	105.72	109.40
3	B	401	NAD	O2A-PA-O1A	3.47	129.40	112.24
3	B	401	NAD	O4B-C4B-C3B	3.46	111.96	105.11
3	B	401	NAD	C2B-C3B-C4B	-3.28	96.27	102.64
3	A	401	NAD	C6N-C5N-C4N	3.25	124.17	119.44
3	A	401	NAD	C4N-C3N-C7N	-3.12	112.70	121.04
3	B	401	NAD	C4N-C3N-C7N	-3.08	112.80	121.04
3	A	401	NAD	O5D-PN-O1N	2.99	120.75	109.07
3	B	401	NAD	O2B-C2B-C3B	2.97	121.44	111.82
3	B	401	NAD	O5D-PN-O1N	2.97	120.66	109.07
3	A	401	NAD	O2B-C2B-C1B	2.95	121.74	110.85
3	A	401	NAD	O2B-C2B-C3B	2.66	120.42	111.82
3	B	401	NAD	O3D-C3D-C4D	-2.65	103.37	111.05
3	A	401	NAD	O2N-PN-O5D	2.47	119.19	107.75
3	B	401	NAD	O4D-C4D-C5D	-2.43	101.39	109.37
3	B	401	NAD	C3B-C2B-C1B	2.42	104.63	100.98
2	A	403	SO4	O3-S-O1	2.37	121.66	109.31
3	A	401	NAD	C3D-C2D-C1D	2.31	104.46	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	NAD	C5B-C4B-C3B	-2.31	106.53	115.18
3	A	401	NAD	C6N-N1N-C2N	-2.30	119.88	121.97
3	A	401	NAD	C5N-C4N-C3N	-2.28	117.65	120.34
3	B	401	NAD	C1B-N9A-C4A	-2.27	122.65	126.64

There are no chirality outliers.

All (10) 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	A	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	C2D-C1D-N1N-C6N
4	A	402	OXM	N1-C1-C2-O3
4	A	402	OXM	N1-C1-C2-O2
3	B	401	NAD	C2D-C1D-N1N-C2N
3	A	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	O4B-C4B-C5B-O5B

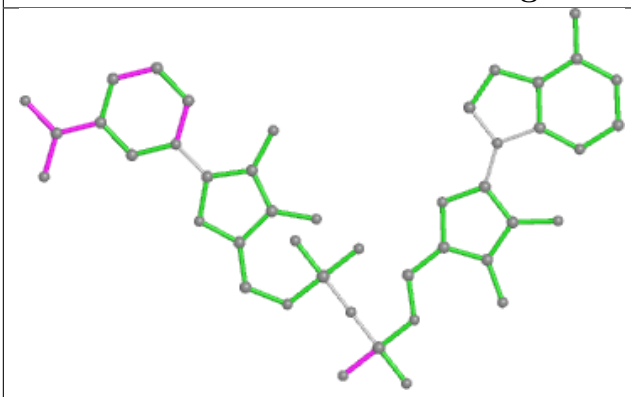
There are no ring outliers.

2 monomers are involved in 3 short contacts:

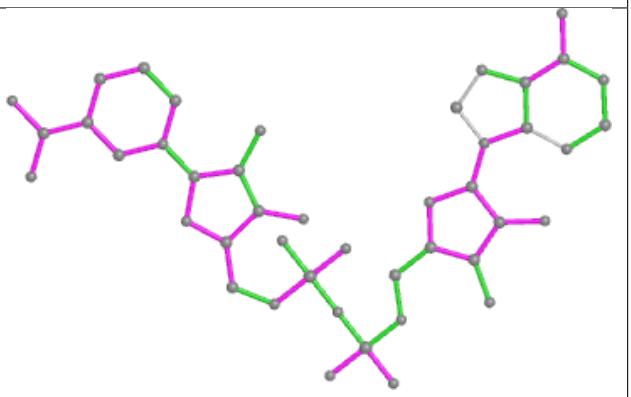
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	NAD	2	0
3	A	401	NAD	1	0

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.

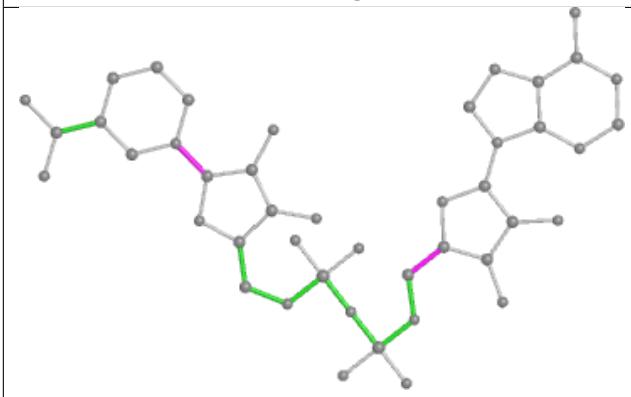
Ligand NAD B 401



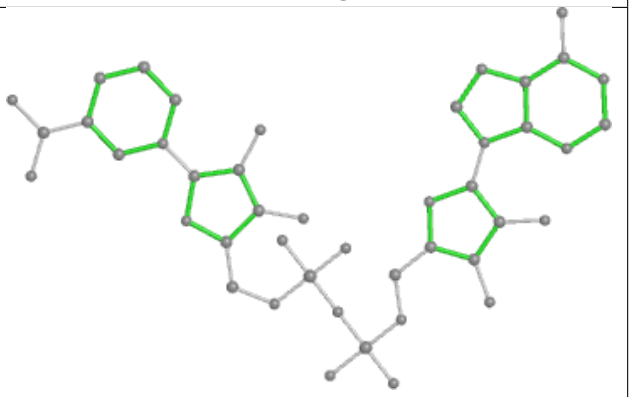
Bond lengths



Bond angles

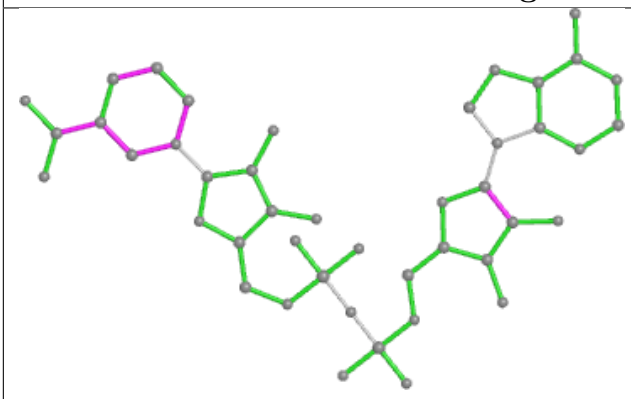


Torsions

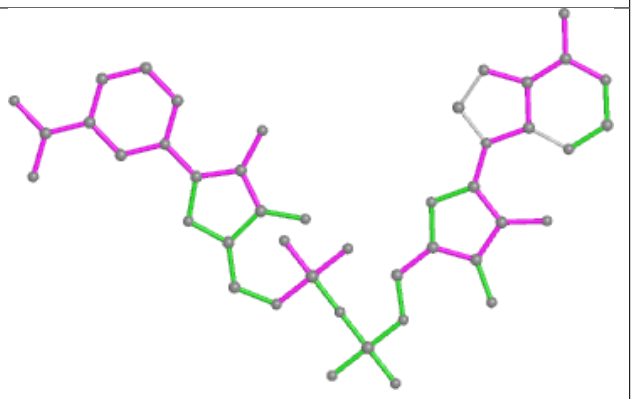


Rings

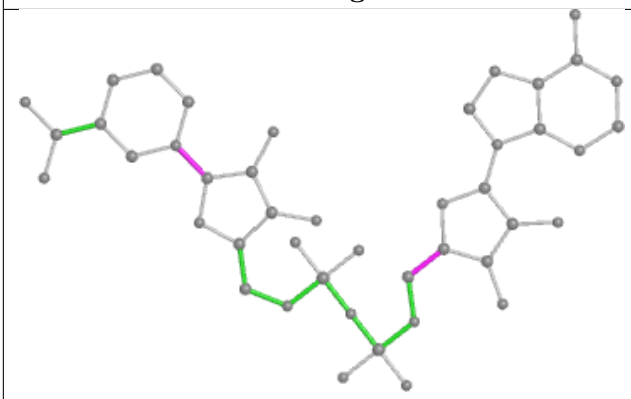
Ligand NAD A 401



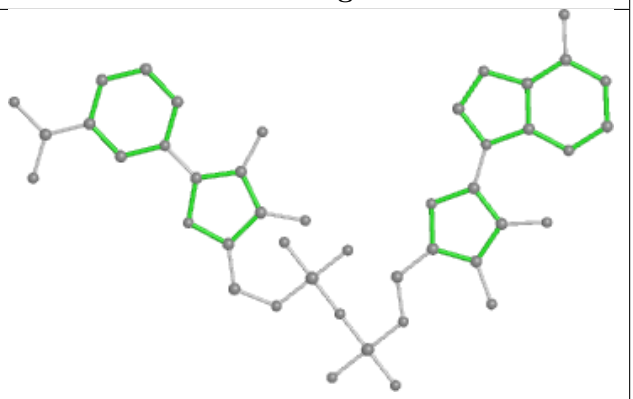
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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.