



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:21 AM UTC

PDB ID : 1O6Z / pdb_00001o6z
Title : 1.95 Å resolution structure of (R207S,R292S) mutant of malate dehydrogenase from the halophilic archaeon Haloarcula marismortui (holo form)
Authors : Irimia, A.; Ebel, C.; Madern, D.; Richard, S.B.; Cosenza, L.W.; Zaccai, G.; Vellieux, F.M.D.
Deposited on : 2002-10-22
Resolution : 1.95 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

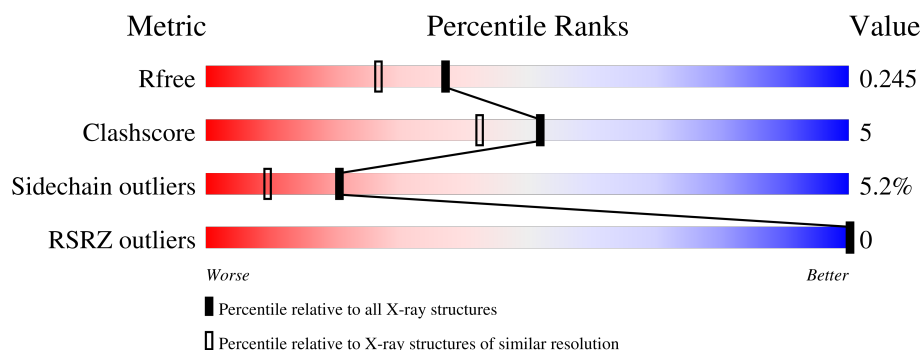
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	 62% 33% 5%
1	B	303	 54% 37% 7% ..
1	C	303	 56% 40% .
1	D	303	 58% 37% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10011 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 MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	4	0
			2326	1427	394	501	4			
1	B	298	Total	C	N	O	S	0	1	0
			2261	1390	379	488	4			
1	C	303	Total	C	N	O	S	0	2	0
			2310	1419	392	495	4			
1	D	298	Total	C	N	O	S	0	0	0
			2253	1386	378	485	4			

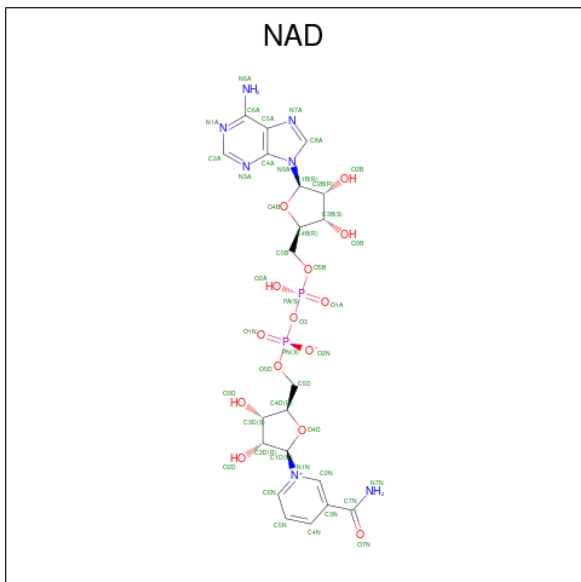
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	ARG	engineered mutation	UNP Q07841
A	292	SER	ARG	engineered mutation	UNP Q07841
B	207	SER	ARG	engineered mutation	UNP Q07841
B	292	SER	ARG	engineered mutation	UNP Q07841
C	207	SER	ARG	engineered mutation	UNP Q07841
C	292	SER	ARG	engineered mutation	UNP Q07841
D	207	SER	ARG	engineered mutation	UNP Q07841
D	292	SER	ARG	engineered mutation	UNP Q07841

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

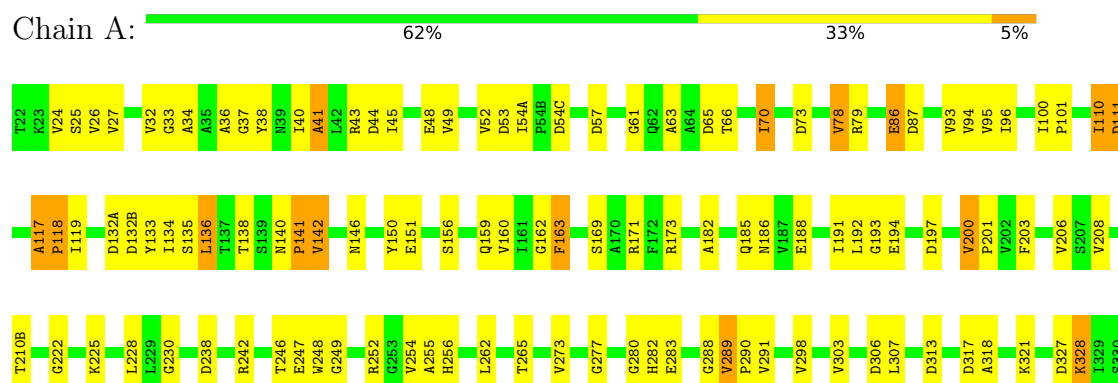
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	160	Total O 160 160	0	0
4	B	170	Total O 170 170	0	0
4	C	166	Total O 166 166	0	0
4	D	181	Total O 181 181	0	0

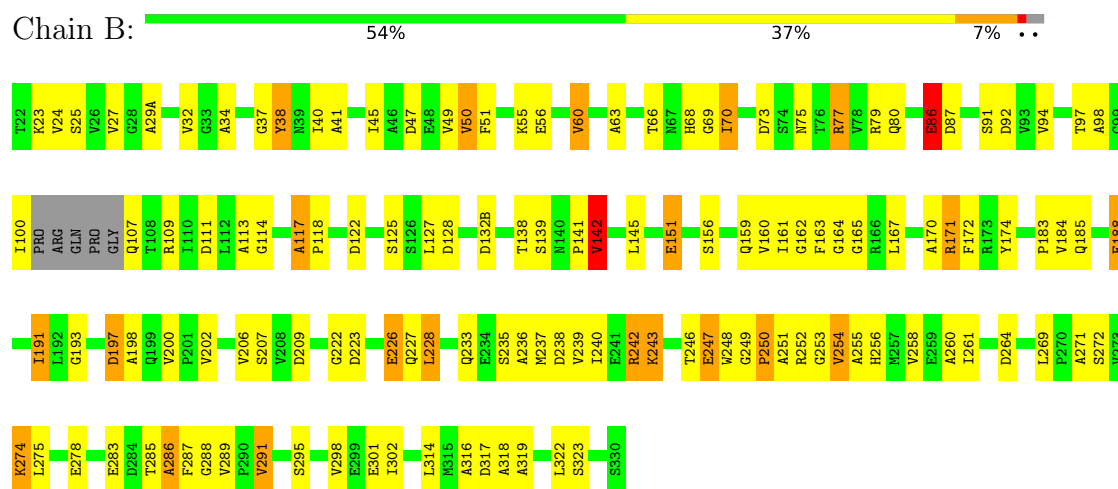
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

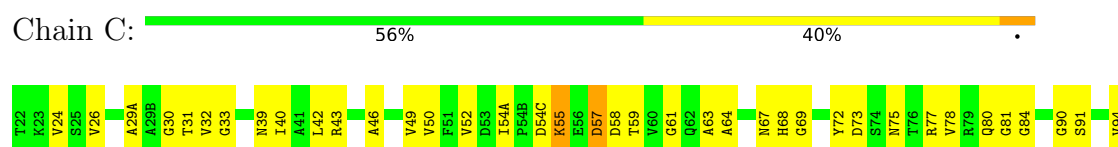
• Molecule 1: MALATE DEHYDROGENASE

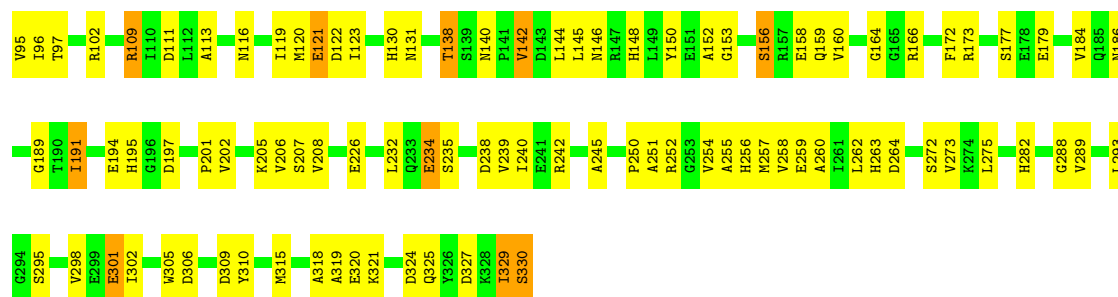


• Molecule 1: MALATE DEHYDROGENASE



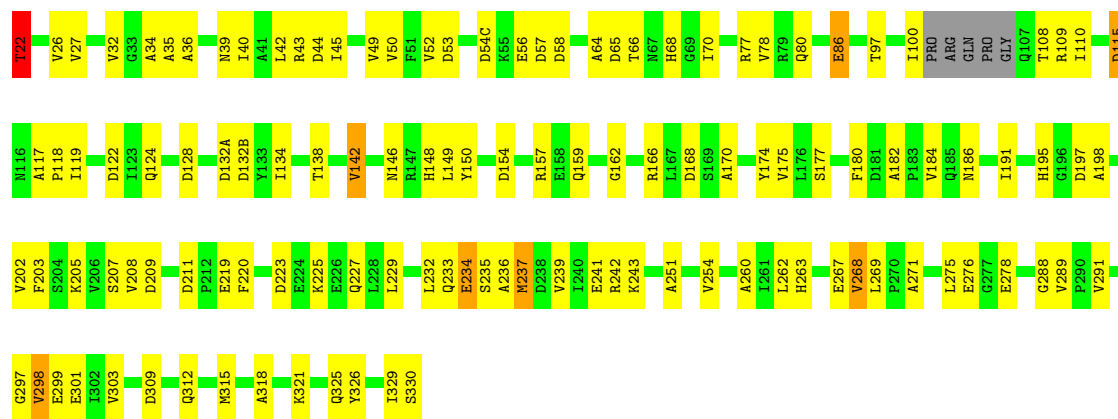
• Molecule 1: MALATE DEHYDROGENASE





• Molecule 1: MALATE DEHYDROGENASE

Chain D: 58% 37%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.64Å 114.42Å 124.87Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	12.00 – 1.95 12.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	78.8 (12.00-1.95) 67.7 (12.00-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.263 (Not available) , 0.245	Depositor DCC
R_{free} test set	5076 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10011	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	2.20	89/2363 (3.8%)	1.58	13/3210 (0.4%)
1	B	2.34	104/2295 (4.5%)	1.65	28/3116 (0.9%)
1	C	2.32	106/2347 (4.5%)	1.60	24/3188 (0.8%)
1	D	2.28	98/2287 (4.3%)	1.61	20/3105 (0.6%)
All	All	2.28	397/9292 (4.3%)	1.61	85/12619 (0.7%)

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	C	0	1

All (397) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	ALA	CA-CB	-11.39	1.35	1.53
1	C	40	ILE	C-O	-10.59	1.11	1.24
1	B	291	VAL	C-O	-10.52	1.13	1.24
1	B	288	GLY	C-O	-10.37	1.15	1.24
1	B	50	VAL	CA-CB	-10.34	1.41	1.54
1	A	256	HIS	C-O	10.03	1.35	1.24
1	C	80	GLN	C-O	-9.93	1.11	1.23
1	C	152	ALA	CA-CB	9.88	1.69	1.53
1	D	182	ALA	CA-CB	-9.82	1.42	1.53
1	B	249	GLY	C-O	9.45	1.36	1.24
1	D	288	GLY	C-O	-9.38	1.16	1.24
1	D	39	ASN	C-O	-9.35	1.13	1.24
1	C	54(A)	ILE	CA-CB	9.31	1.66	1.54
1	B	45	ILE	CA-CB	-9.24	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	LEU	C-O	9.23	1.34	1.24
1	C	24	VAL	CA-CB	-9.07	1.42	1.54
1	C	68	HIS	C-O	9.00	1.34	1.24
1	D	64	ALA	CA-CB	-9.00	1.39	1.53
1	D	40	ILE	CA-CB	8.99	1.65	1.54
1	D	36	ALA	CA-CB	8.93	1.67	1.53
1	D	49	VAL	C-O	-8.83	1.14	1.24
1	A	54(A)	ILE	CA-CB	8.77	1.65	1.54
1	A	26	VAL	CA-CB	-8.76	1.43	1.54
1	B	68	HIS	C-O	8.73	1.34	1.24
1	D	42	LEU	CA-C	8.71	1.64	1.52
1	B	256	HIS	C-O	8.69	1.34	1.24
1	A	169	SER	C-O	-8.69	1.13	1.24
1	B	45	ILE	C-O	8.62	1.33	1.24
1	D	269	LEU	C-O	-8.62	1.13	1.24
1	B	161	ILE	C-O	-8.57	1.14	1.24
1	C	113	ALA	CA-CB	-8.48	1.40	1.53
1	C	235	SER	C-O	-8.47	1.14	1.24
1	B	317	ASP	C-O	-8.38	1.14	1.24
1	A	182	ALA	CA-CB	-8.29	1.42	1.53
1	C	250	PRO	C-O	-8.28	1.14	1.24
1	D	309	ASP	C-O	-8.26	1.14	1.24
1	D	237	MET	SD-CE	-8.23	1.58	1.79
1	D	36	ALA	C-O	-8.16	1.14	1.24
1	C	256	HIS	C-O	8.13	1.33	1.24
1	C	159	GLN	C-O	-8.10	1.13	1.24
1	C	234	GLU	CA-C	8.04	1.63	1.52
1	D	58	ASP	C-O	-8.03	1.14	1.24
1	B	60	VAL	C-O	-8.02	1.14	1.24
1	D	168	ASP	C-O	-8.02	1.14	1.24
1	B	40	ILE	C-O	-7.96	1.15	1.24
1	D	260	ALA	CA-C	7.95	1.63	1.52
1	C	251	ALA	N-CA	-7.87	1.37	1.46
1	A	210(B)	THR	CA-C	-7.77	1.42	1.53
1	D	198	ALA	CA-CB	7.77	1.62	1.52
1	A	298	VAL	CA-CB	-7.75	1.45	1.54
1	C	121	GLU	C-O	-7.74	1.14	1.24
1	A	307	LEU	C-O	-7.71	1.14	1.23
1	A	186	ASN	C-O	7.70	1.34	1.23
1	C	202	VAL	CA-CB	-7.67	1.44	1.54
1	C	49	VAL	C-O	7.66	1.32	1.24
1	C	240	ILE	C-O	-7.66	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	VAL	CA-CB	-7.64	1.46	1.55
1	B	79	ARG	CA-C	-7.61	1.43	1.52
1	D	132(A)	ASP	C-O	7.57	1.30	1.23
1	D	184	VAL	CA-CB	7.53	1.65	1.54
1	A	87	ASP	C-O	7.51	1.33	1.24
1	B	240	ILE	C-O	-7.51	1.15	1.24
1	C	145	LEU	C-O	-7.50	1.15	1.24
1	B	250	PRO	CA-C	-7.49	1.41	1.52
1	B	285	THR	CA-CB	7.47	1.66	1.53
1	A	254	VAL	CA-C	-7.47	1.43	1.52
1	A	289	VAL	CA-C	-7.44	1.45	1.52
1	C	239	VAL	C-O	-7.38	1.15	1.24
1	C	96	ILE	C-O	-7.35	1.16	1.24
1	C	263	HIS	C-O	7.35	1.34	1.23
1	C	252	ARG	C-O	-7.34	1.15	1.24
1	C	120	MET	SD-CE	7.33	1.97	1.79
1	B	286	ALA	C-O	7.33	1.32	1.23
1	B	41	ALA	CA-CB	7.28	1.64	1.53
1	D	45	ILE	C-O	-7.27	1.16	1.24
1	B	226	GLU	CA-C	-7.23	1.43	1.52
1	A	171	ARG	C-O	7.20	1.32	1.24
1	D	43	ARG	N-CA	-7.20	1.36	1.46
1	C	289	VAL	CA-C	-7.19	1.45	1.52
1	D	174	TYR	C-O	-7.19	1.15	1.24
1	A	252	ARG	C-O	-7.16	1.15	1.24
1	C	258	VAL	CA-CB	-7.16	1.45	1.54
1	C	319	ALA	CA-CB	7.16	1.64	1.53
1	C	94	VAL	CA-CB	-7.13	1.45	1.54
1	A	63	ALA	CA-CB	7.12	1.64	1.53
1	C	72	TYR	CZ-OH	7.09	1.52	1.38
1	B	191	ILE	C-O	-7.09	1.16	1.24
1	B	41	ALA	C-O	-7.01	1.15	1.24
1	B	117	ALA	CA-C	6.98	1.61	1.52
1	A	283	GLU	CA-C	-6.97	1.44	1.52
1	C	205	LYS	N-CA	6.95	1.54	1.46
1	D	35	ALA	C-O	-6.94	1.16	1.24
1	B	174	TYR	C-O	6.94	1.32	1.24
1	C	315	MET	C-O	6.88	1.32	1.24
1	D	297	GLY	C-O	6.85	1.33	1.23
1	D	32	VAL	CA-CB	-6.81	1.45	1.54
1	B	261	ILE	CA-CB	-6.80	1.45	1.54
1	A	48	GLU	CA-C	-6.80	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	VAL	C-O	-6.80	1.16	1.24
1	C	260	ALA	C-O	-6.75	1.15	1.24
1	B	66	THR	N-CA	-6.69	1.38	1.46
1	C	30	GLY	C-O	6.68	1.31	1.23
1	A	41	ALA	CA-CB	6.67	1.63	1.53
1	D	278	GLU	N-CA	6.67	1.54	1.46
1	D	186	ASN	CA-C	6.67	1.61	1.52
1	D	205	LYS	CG-CD	6.66	1.72	1.52
1	A	118	PRO	C-O	-6.66	1.16	1.24
1	C	206	VAL	C-O	-6.65	1.16	1.24
1	D	108	THR	CA-CB	-6.65	1.42	1.53
1	B	236	ALA	CA-CB	-6.63	1.42	1.53
1	B	47	ASP	CA-C	6.62	1.61	1.52
1	B	160	VAL	CA-CB	6.62	1.62	1.53
1	B	202	VAL	C-O	6.61	1.31	1.24
1	D	236	ALA	CA-CB	-6.60	1.42	1.53
1	A	33	GLY	C-O	6.58	1.31	1.23
1	D	220	PHE	CA-C	6.57	1.60	1.52
1	A	273	VAL	CA-CB	6.56	1.65	1.55
1	B	34	ALA	C-O	6.53	1.31	1.24
1	D	202	VAL	CA-CB	-6.53	1.45	1.54
1	B	24	VAL	CA-CB	-6.52	1.46	1.54
1	A	150	TYR	C-O	-6.52	1.16	1.24
1	C	251	ALA	C-O	-6.50	1.16	1.24
1	D	97	THR	CA-CB	6.49	1.63	1.53
1	C	320	GLU	C-O	-6.47	1.16	1.24
1	D	65	ASP	CA-C	6.46	1.61	1.52
1	C	189	GLY	C-O	-6.44	1.16	1.24
1	C	245	ALA	CA-C	-6.44	1.44	1.52
1	B	255	ALA	CA-C	6.43	1.61	1.52
1	C	50	VAL	CA-CB	-6.40	1.46	1.54
1	D	299	GLU	CD-OE2	-6.40	1.13	1.25
1	A	151	GLU	N-CA	6.39	1.54	1.46
1	A	192	LEU	CA-C	6.39	1.62	1.53
1	D	168	ASP	CA-CB	6.39	1.63	1.53
1	A	32	VAL	CA-CB	6.38	1.62	1.54
1	B	92	ASP	CA-C	-6.38	1.44	1.52
1	B	138	THR	CB-CG2	6.37	1.73	1.52
1	B	251	ALA	N-CA	6.37	1.54	1.46
1	B	66	THR	C-O	-6.36	1.16	1.24
1	C	186	ASN	CA-C	6.34	1.61	1.52
1	B	206	VAL	CA-C	6.33	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	VAL	C-O	-6.33	1.16	1.23
1	D	263	HIS	C-O	-6.32	1.15	1.24
1	C	40	ILE	N-CA	-6.29	1.38	1.46
1	B	94	VAL	C-O	6.28	1.30	1.24
1	A	94	VAL	C-O	-6.25	1.17	1.24
1	A	303	VAL	N-CA	-6.25	1.38	1.46
1	B	222	GLY	C-O	-6.24	1.16	1.23
1	B	272	SER	C-O	-6.21	1.16	1.24
1	A	246	THR	N-CA	-6.20	1.38	1.46
1	C	208	VAL	CA-C	-6.19	1.45	1.52
1	C	31	THR	CA-C	6.16	1.60	1.52
1	B	165	GLY	CA-C	6.14	1.59	1.52
1	C	184	VAL	CA-CB	6.14	1.62	1.54
1	A	24	VAL	CA-CB	-6.13	1.46	1.54
1	B	226	GLU	N-CA	6.13	1.53	1.46
1	C	111	ASP	CB-CG	6.13	1.67	1.52
1	A	277	GLY	C-O	-6.12	1.15	1.24
1	B	252	ARG	C-O	-6.11	1.16	1.24
1	A	119	ILE	CA-CB	6.10	1.62	1.54
1	A	95	VAL	C-O	-6.10	1.17	1.24
1	C	26	VAL	CA-CB	-6.10	1.46	1.53
1	C	42	LEU	C-O	-6.10	1.16	1.24
1	D	209	ASP	C-O	-6.09	1.15	1.23
1	B	286	ALA	CA-CB	-6.08	1.43	1.53
1	C	97	THR	CA-CB	6.08	1.63	1.53
1	D	219	GLU	C-O	6.07	1.31	1.24
1	B	302	ILE	C-O	-6.06	1.17	1.24
1	B	171	ARG	NE-CZ	6.06	1.39	1.33
1	B	289	VAL	CA-C	6.06	1.57	1.52
1	B	253	GLY	N-CA	-6.06	1.38	1.45
1	C	95	VAL	CA-C	6.05	1.60	1.52
1	B	243	LYS	N-CA	-6.04	1.39	1.46
1	C	55	LYS	CB-CG	6.03	1.70	1.52
1	C	54(A)	ILE	N-CA	6.02	1.53	1.46
1	A	283	GLU	C-O	-6.02	1.16	1.23
1	B	261	ILE	C-O	-6.01	1.17	1.24
1	B	242	ARG	CA-C	6.00	1.60	1.52
1	C	184	VAL	C-O	-5.99	1.16	1.24
1	C	282	HIS	C-O	-5.99	1.16	1.23
1	C	160	VAL	C-O	-5.99	1.17	1.24
1	A	49	VAL	CA-CB	-5.98	1.47	1.54
1	B	111	ASP	CA-C	5.98	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	GLU	CA-C	5.98	1.60	1.52
1	B	298	VAL	CA-C	5.97	1.59	1.53
1	C	52	VAL	CA-C	5.96	1.59	1.52
1	D	43	ARG	CA-C	5.95	1.60	1.52
1	C	298	VAL	CA-C	-5.94	1.46	1.52
1	B	127	LEU	N-CA	5.94	1.53	1.46
1	C	208	VAL	CA-CB	-5.93	1.46	1.54
1	C	258	VAL	N-CA	-5.93	1.39	1.46
1	D	149	LEU	N-CA	5.92	1.53	1.46
1	D	298	VAL	CA-C	5.90	1.59	1.52
1	A	298	VAL	C-O	-5.89	1.17	1.24
1	B	254	VAL	CB-CG2	-5.89	1.33	1.52
1	D	268	VAL	CA-CB	5.88	1.61	1.54
1	D	271	ALA	CA-CB	-5.87	1.44	1.53
1	C	302	ILE	CA-CB	-5.87	1.47	1.54
1	D	162	GLY	CA-C	5.86	1.56	1.52
1	C	302	ILE	CA-C	5.86	1.60	1.52
1	D	27	VAL	CA-CB	-5.86	1.47	1.54
1	D	237	MET	CG-SD	5.84	1.95	1.80
1	A	65	ASP	C-O	5.84	1.31	1.24
1	A	289	VAL	CA-CB	-5.83	1.46	1.54
1	B	142	VAL	CA-CB	5.83	1.61	1.54
1	D	312	GLN	N-CA	5.82	1.53	1.46
1	A	57	ASP	C-O	5.81	1.30	1.24
1	A	53	ASP	C-O	-5.81	1.17	1.23
1	C	252	ARG	N-CA	5.79	1.53	1.46
1	A	101	PRO	CA-C	5.79	1.59	1.52
1	B	87	ASP	CA-C	5.78	1.60	1.52
1	D	276	GLU	C-O	-5.78	1.16	1.23
1	D	26	VAL	C-O	5.76	1.30	1.24
1	C	144	LEU	C-O	5.75	1.30	1.24
1	A	160	VAL	CA-CB	-5.75	1.47	1.53
1	B	233	GLN	C-O	-5.75	1.17	1.24
1	D	170	ALA	C-O	-5.74	1.17	1.24
1	B	32	VAL	CA-C	-5.72	1.45	1.52
1	A	208	VAL	CA-CB	-5.71	1.47	1.54
1	B	198	ALA	CA-CB	-5.71	1.45	1.52
1	C	254	VAL	CA-C	-5.71	1.46	1.52
1	A	36	ALA	N-CA	5.71	1.53	1.46
1	C	324	ASP	CB-CG	5.70	1.66	1.52
1	C	138	THR	CA-CB	-5.69	1.44	1.53
1	D	211	ASP	N-CA	5.69	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	GLY	C-O	5.69	1.31	1.24
1	C	235	SER	N-CA	-5.69	1.39	1.46
1	C	64	ALA	CA-CB	5.68	1.62	1.53
1	B	160	VAL	C-O	5.68	1.32	1.23
1	A	317	ASP	CA-C	-5.67	1.45	1.52
1	B	68	HIS	CA-C	-5.67	1.45	1.52
1	C	301	GLU	N-CA	5.67	1.52	1.46
1	C	123	ILE	CA-CB	-5.67	1.48	1.54
1	A	38	TYR	CZ-OH	5.67	1.50	1.38
1	A	146	ASN	C-O	5.67	1.30	1.24
1	D	275	LEU	CA-C	5.67	1.59	1.52
1	D	303	VAL	C-O	5.66	1.30	1.24
1	D	191	ILE	CA-CB	-5.66	1.47	1.54
1	A	25	SER	CA-C	5.65	1.59	1.52
1	A	201	PRO	C-O	-5.64	1.17	1.23
1	C	77	ARG	CD-NE	5.62	1.54	1.46
1	A	206	VAL	C-O	-5.62	1.18	1.24
1	A	101	PRO	C-O	5.62	1.30	1.23
1	C	319	ALA	C-O	5.62	1.30	1.24
1	B	188	GLU	N-CA	-5.62	1.39	1.46
1	A	34	ALA	C-O	-5.61	1.17	1.24
1	C	257	MET	SD-CE	-5.60	1.65	1.79
1	C	232	LEU	C-O	-5.60	1.17	1.24
1	A	70	ILE	C-O	5.59	1.32	1.24
1	B	183	PRO	C-O	-5.59	1.16	1.23
1	D	289	VAL	N-CA	-5.58	1.41	1.46
1	C	54(C)	ASP	C-O	-5.58	1.16	1.24
1	A	96	ILE	C-O	-5.57	1.18	1.24
1	A	298	VAL	CA-C	5.57	1.59	1.52
1	D	315	MET	CA-C	5.56	1.60	1.52
1	B	69	GLY	C-O	-5.56	1.17	1.24
1	C	177	SER	C-O	-5.55	1.17	1.24
1	B	25	SER	C-O	5.54	1.30	1.23
1	D	325	GLN	C-O	-5.54	1.17	1.24
1	A	146	ASN	CG-OD1	5.54	1.34	1.23
1	A	162	GLY	CA-C	-5.54	1.48	1.52
1	C	305	TRP	C-O	5.53	1.30	1.23
1	B	60	VAL	N-CA	-5.52	1.40	1.46
1	D	150	TYR	CA-C	-5.52	1.45	1.52
1	D	254	VAL	CA-CB	-5.52	1.48	1.54
1	B	264	ASP	C-O	-5.52	1.16	1.23
1	A	117	ALA	CA-CB	-5.51	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29(A)	ALA	C-O	5.51	1.31	1.24
1	A	140	ASN	CA-C	-5.51	1.45	1.52
1	A	133	TYR	N-CA	-5.50	1.39	1.46
1	A	37	GLY	C-O	-5.49	1.17	1.23
1	B	139	SER	N-CA	-5.49	1.39	1.46
1	B	70	ILE	CA-CB	5.47	1.60	1.54
1	A	45	ILE	CA-CB	5.47	1.61	1.54
1	A	135	SER	CA-C	-5.47	1.46	1.52
1	A	291	VAL	N-CA	5.46	1.52	1.46
1	C	295	SER	C-O	-5.46	1.17	1.24
1	D	299	GLU	N-CA	-5.46	1.39	1.46
1	A	93	VAL	CA-C	-5.45	1.45	1.52
1	C	153	GLY	C-O	5.45	1.28	1.23
1	C	327	ASP	CA-C	5.45	1.60	1.52
1	B	271	ALA	CA-CB	-5.45	1.44	1.53
1	D	118	PRO	CA-C	5.44	1.60	1.52
1	A	134	ILE	N-CA	-5.44	1.39	1.46
1	B	162	GLY	CA-C	5.42	1.56	1.52
1	C	146	ASN	CG-OD1	5.42	1.33	1.23
1	B	286	ALA	N-CA	5.42	1.52	1.46
1	C	33	GLY	CA-C	5.41	1.59	1.51
1	A	78	VAL	CA-CB	5.41	1.61	1.54
1	D	54(C)	ASP	CA-C	5.40	1.60	1.52
1	B	63	ALA	CA-CB	-5.40	1.44	1.53
1	A	159	GLN	C-O	-5.40	1.17	1.24
1	C	116	ASN	C-O	-5.39	1.17	1.24
1	B	239	VAL	N-CA	-5.38	1.40	1.46
1	A	52	VAL	CA-CB	5.38	1.61	1.54
1	A	63	ALA	C-O	5.38	1.30	1.24
1	D	64	ALA	CA-C	-5.38	1.46	1.52
1	B	27	VAL	CA-CB	-5.37	1.47	1.53
1	B	283	GLU	C-O	5.37	1.31	1.23
1	B	66	THR	CA-CB	5.36	1.61	1.53
1	C	119	ILE	C-O	-5.35	1.18	1.24
1	D	56	GLU	N-CA	-5.35	1.39	1.46
1	B	316	ALA	CA-C	-5.35	1.46	1.52
1	A	100	ILE	CA-CB	-5.34	1.47	1.54
1	D	119	ILE	C-O	5.34	1.30	1.24
1	C	262	LEU	CA-C	-5.34	1.45	1.52
1	C	318	ALA	CA-CB	-5.34	1.45	1.53
1	D	318	ALA	C-O	-5.33	1.17	1.24
1	A	191	ILE	CA-C	5.33	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	MET	C-O	-5.33	1.17	1.24
1	D	44	ASP	C-O	5.33	1.30	1.23
1	B	185	GLN	CB-CG	5.32	1.68	1.52
1	C	69	GLY	CA-C	5.32	1.58	1.52
1	C	255	ALA	CA-CB	5.32	1.61	1.53
1	A	134	ILE	CA-CB	5.32	1.61	1.54
1	C	207	SER	C-O	-5.32	1.17	1.23
1	C	46	ALA	CA-CB	-5.31	1.44	1.53
1	D	203	PHE	C-O	5.31	1.30	1.24
1	A	247	GLU	CD-OE1	5.31	1.35	1.25
1	A	173	ARG	C-O	5.30	1.30	1.24
1	C	275	LEU	CA-C	5.30	1.59	1.52
1	B	132(B)	ASP	C-O	5.28	1.30	1.23
1	C	201	PRO	C-O	-5.28	1.18	1.23
1	D	208	VAL	CA-C	-5.28	1.46	1.52
1	D	34	ALA	N-CA	-5.28	1.40	1.46
1	D	197	ASP	CA-C	5.28	1.59	1.52
1	D	207	SER	C-O	-5.27	1.18	1.24
1	D	100	ILE	CG1-CD1	5.27	1.72	1.51
1	D	134	ILE	CA-CB	5.26	1.60	1.54
1	B	314	LEU	C-O	-5.26	1.17	1.24
1	C	179	GLU	C-O	-5.26	1.17	1.24
1	A	185	GLN	C-O	-5.25	1.17	1.24
1	A	27	VAL	C-O	-5.24	1.18	1.24
1	C	57	ASP	CA-C	5.24	1.59	1.52
1	D	65	ASP	CG-OD2	5.24	1.35	1.25
1	D	234	GLU	CD-OE2	5.23	1.35	1.25
1	A	45	ILE	C-O	-5.22	1.19	1.24
1	A	141	PRO	CB-CG	-5.22	1.30	1.51
1	D	251	ALA	C-O	5.22	1.30	1.24
1	C	306	ASP	CB-CG	5.21	1.65	1.52
1	B	38	TYR	CA-CB	-5.21	1.45	1.53
1	B	51	PHE	C-O	5.20	1.30	1.24
1	C	145	LEU	CG-CD2	5.20	1.69	1.52
1	A	171	ARG	NE-CZ	-5.19	1.27	1.33
1	B	323	SER	CA-C	5.19	1.59	1.52
1	D	154	ASP	CB-CG	5.19	1.65	1.52
1	D	234	GLU	C-O	5.19	1.30	1.24
1	B	235	SER	CA-C	5.19	1.59	1.52
1	C	293	LEU	CA-CB	5.19	1.60	1.53
1	D	157	ARG	C-O	-5.19	1.17	1.24
1	B	75	ASN	C-O	-5.18	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	78	VAL	CA-CB	5.18	1.61	1.54
1	D	208	VAL	C-O	-5.17	1.18	1.24
1	B	32	VAL	CA-CB	-5.16	1.48	1.54
1	D	132(B)	ASP	C-O	5.15	1.29	1.24
1	D	227	GLN	N-CA	-5.15	1.40	1.46
1	B	184	VAL	C-O	-5.15	1.17	1.24
1	B	60	VAL	CA-CB	5.15	1.60	1.54
1	B	226	GLU	C-O	-5.14	1.18	1.24
1	C	288	GLY	C-O	5.14	1.29	1.24
1	A	318	ALA	CA-CB	5.14	1.61	1.53
1	B	316	ALA	CA-CB	-5.13	1.45	1.53
1	D	77	ARG	C-O	-5.13	1.17	1.24
1	C	61	GLY	C-O	-5.12	1.17	1.23
1	D	175	VAL	CB-CG1	-5.12	1.35	1.52
1	C	173	ARG	CG-CD	-5.12	1.37	1.52
1	C	259	GLU	CD-OE2	5.12	1.35	1.25
1	B	60	VAL	CA-C	5.11	1.59	1.52
1	D	180	PHE	N-CA	5.11	1.52	1.46
1	A	38	TYR	N-CA	-5.10	1.40	1.46
1	C	84	GLY	C-O	-5.10	1.19	1.23
1	A	230	GLY	C-O	-5.10	1.17	1.23
1	B	247	GLU	CA-C	5.09	1.59	1.52
1	D	124	GLN	CD-OE1	5.09	1.33	1.23
1	B	128	ASP	C-O	5.09	1.30	1.24
1	A	265	THR	CA-CB	5.09	1.61	1.53
1	A	282	HIS	C-O	5.08	1.30	1.23
1	B	240	ILE	CA-CB	5.08	1.60	1.54
1	D	68	HIS	CA-C	5.08	1.59	1.52
1	C	309	ASP	N-CA	5.07	1.52	1.46
1	D	65	ASP	C-O	5.07	1.30	1.24
1	D	243	LYS	CA-CB	-5.07	1.45	1.53
1	C	150	TYR	C-O	5.07	1.29	1.24
1	C	272	SER	N-CA	-5.05	1.40	1.46
1	A	40	ILE	N-CA	-5.05	1.40	1.46
1	B	319	ALA	C-O	-5.05	1.18	1.24
1	A	163	PHE	CE1-CZ	5.04	1.53	1.38
1	C	29(A)	ALA	CA-C	5.03	1.59	1.52
1	A	288	GLY	C-O	5.03	1.30	1.23
1	D	326	TYR	N-CA	-5.02	1.40	1.46
1	D	321	LYS	C-O	-5.02	1.18	1.24
1	C	102	ARG	CA-C	5.02	1.59	1.52
1	D	227	GLN	CG-CD	5.02	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	VAL	CA-CB	5.02	1.61	1.54
1	D	299	GLU	CA-C	-5.01	1.46	1.52
1	D	53	ASP	CA-C	-5.01	1.46	1.52
1	D	267	GLU	C-O	-5.01	1.17	1.23
1	B	274	LYS	C-O	-5.01	1.18	1.23

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29(A)	ALA	N-CA-C	8.80	123.43	112.87
1	C	142	VAL	N-CA-C	8.56	118.64	110.42
1	C	59	THR	N-CA-C	-8.02	102.62	111.36
1	C	239	VAL	N-CA-C	7.94	117.99	110.53
1	D	239	VAL	N-CA-C	-7.63	104.35	111.45
1	B	164	GLY	CA-C-N	7.29	128.20	120.03
1	B	164	GLY	C-N-CA	7.29	128.20	120.03
1	B	92	ASP	N-CA-C	-7.27	104.04	113.12
1	A	111	ASP	N-CA-C	-7.16	103.56	111.36
1	C	153	GLY	N-CA-C	-6.84	103.20	112.57
1	B	142	VAL	CB-CA-C	-6.82	102.80	112.22
1	A	44	ASP	CA-C-N	6.82	129.96	121.85
1	A	44	ASP	C-N-CA	6.82	129.96	121.85
1	C	96	ILE	N-CA-C	6.69	117.75	107.99
1	B	228	LEU	N-CA-C	-6.54	103.99	112.23
1	C	173	ARG	N-CA-C	-6.50	104.27	111.36
1	B	287	PHE	CA-C-N	6.46	126.80	120.98
1	B	287	PHE	C-N-CA	6.46	126.80	120.98
1	D	56	GLU	N-CA-C	-6.40	104.38	111.36
1	B	98	ALA	N-CA-C	6.25	118.62	110.43
1	C	58	ASP	N-CA-C	-6.25	104.55	111.36
1	B	318	ALA	N-CA-C	6.24	118.60	111.11
1	B	97	THR	OG1-CB-CG2	-6.20	96.90	109.30
1	D	235	SER	N-CA-C	-6.15	104.65	111.36
1	C	282	HIS	N-CA-C	6.14	119.50	109.24
1	C	122	ASP	N-CA-C	6.13	117.76	111.14
1	D	52	VAL	CB-CA-C	-6.09	101.55	110.62
1	C	201	PRO	N-CD-CG	-6.01	94.19	103.20
1	D	22	THR	OG1-CB-CG2	-5.93	97.43	109.30
1	D	195	HIS	CA-CB-CG	-5.93	107.87	113.80
1	B	66	THR	OG1-CB-CG2	-5.87	97.56	109.30
1	D	118	PRO	N-CD-CG	-5.87	94.40	103.20
1	C	156	SER	N-CA-C	5.83	118.28	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ASP	N-CA-C	5.80	119.54	112.23
1	C	63	ALA	N-CA-C	-5.74	104.94	111.14
1	B	223	ASP	N-CA-C	5.74	117.53	111.28
1	D	288	GLY	N-CA-C	5.69	119.84	110.97
1	A	27	VAL	CA-C-N	5.67	129.85	122.26
1	A	27	VAL	C-N-CA	5.67	129.85	122.26
1	C	158	GLU	N-CA-C	5.64	118.19	111.71
1	C	81	GLY	CA-C-N	5.63	127.44	122.43
1	C	81	GLY	C-N-CA	5.63	127.44	122.43
1	C	142	VAL	CB-CA-C	-5.57	104.84	111.97
1	D	146	ASN	N-CA-C	5.55	117.01	111.07
1	B	248	TRP	N-CA-C	-5.49	105.37	111.36
1	C	75	ASN	N-CA-C	5.49	119.84	113.20
1	D	289	VAL	CB-CA-C	5.47	115.80	109.89
1	A	142	VAL	CB-CA-C	-5.46	104.87	112.02
1	B	122	ASP	N-CA-C	-5.45	105.25	111.14
1	B	209	ASP	N-CA-C	-5.41	105.31	112.24
1	C	264	ASP	CB-CA-C	-5.41	104.21	111.89
1	B	161	ILE	N-CA-C	5.40	116.08	108.36
1	A	94	VAL	N-CA-C	5.39	115.72	108.17
1	C	164	GLY	CA-C-N	5.35	126.03	120.03
1	C	164	GLY	C-N-CA	5.35	126.03	120.03
1	D	115	ASP	N-CA-C	-5.35	104.87	111.40
1	B	160	VAL	CA-C-O	-5.35	115.17	121.64
1	B	37	GLY	N-CA-C	-5.34	106.24	113.24
1	C	43[A]	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	C	43[B]	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	B	49	VAL	N-CA-CB	5.33	119.07	111.82
1	B	260	ALA	N-CA-C	-5.29	105.69	111.82
1	D	177	SER	CA-CB-OG	5.25	121.60	111.10
1	B	86	GLU	N-CA-C	-5.24	105.74	111.82
1	A	255	ALA	N-CA-C	5.24	116.99	111.28
1	A	252	ARG	CA-C-N	5.23	125.79	119.98
1	A	252	ARG	C-N-CA	5.23	125.79	119.98
1	A	262	LEU	N-CA-C	5.20	117.02	111.36
1	B	60	VAL	CA-C-N	5.19	126.88	120.34
1	B	60	VAL	C-N-CA	5.19	126.88	120.34
1	D	166	ARG	N-CA-C	-5.19	105.62	111.28
1	B	142	VAL	N-CA-CB	5.19	118.36	110.58
1	D	142	VAL	N-CA-C	5.16	115.93	110.72
1	D	262	LEU	N-CA-C	5.16	116.98	111.36
1	C	245	ALA	CB-CA-C	-5.16	100.16	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	ASP	N-CA-C	-5.12	104.63	111.24
1	B	258	VAL	N-CA-C	5.12	115.84	110.62
1	D	162	GLY	O-C-N	-5.11	119.67	123.61
1	B	114	GLY	CA-C-O	-5.11	114.68	120.30
1	A	222	GLY	N-CA-C	-5.10	106.61	112.73
1	B	295	SER	N-CA-C	5.09	118.26	111.75
1	D	138	THR	CA-C-N	5.08	129.34	121.26
1	D	138	THR	C-N-CA	5.08	129.34	121.26
1	A	222	GLY	CA-C-O	-5.03	115.57	120.75
1	D	27	VAL	N-CA-C	-5.02	101.18	108.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	166	ARG	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	2326	0	2170	24	0
1	B	2261	0	2113	33	0
1	C	2310	0	2164	19	0
1	D	2253	0	2110	17	0
2	A	2	0	0	2	0
2	B	2	0	0	1	0
2	C	2	0	0	1	0
2	D	2	0	0	1	0
3	A	44	0	26	1	0
3	B	44	0	25	1	0
3	C	44	0	25	1	0
3	D	44	0	26	0	0
4	A	160	0	0	8	0
4	B	170	0	0	6	0
4	C	166	0	0	4	0
4	D	181	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10011	0	8659	92	0

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 5.

All (92) 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:291:VAL:HB	4:B:2135:HOH:O	1.55	1.05
1:A:54(C)[B]:ASP:OD1	4:A:2016:HOH:O	1.81	0.95
1:B:77:ARG:HA	1:B:77:ARG:HE	1.36	0.90
1:D:117:ALA:HB1	1:D:148:HIS:CD2	2.15	0.81
2:C:1007:CL:CL	4:D:2030:HOH:O	2.49	0.67
1:A:43[B]:ARG:NH2	4:A:2009:HOH:O	2.25	0.66
1:D:22:THR:HG22	4:D:2046:HOH:O	1.94	0.66
1:A:73:ASP:OD2	2:B:1006:CL:CL	2.51	0.65
1:C:130:HIS:ND1	4:C:2060:HOH:O	2.30	0.64
1:A:194:GLU:OE1	1:A:321:LYS:NZ	2.31	0.62
3:B:3002:NAD:N1A	4:B:2166:HOH:O	2.31	0.61
1:B:250:PRO:O	1:B:254:VAL:HG23	2.02	0.60
1:A:238:ASP:O	1:A:242:ARG:HB2	2.03	0.59
1:A:328:LYS:NZ	4:A:2155:HOH:O	2.32	0.57
1:B:286:ALA:O	1:B:322:LEU:HD13	2.04	0.57
1:C:91:SER:H	1:C:131:ASN:HD21	1.51	0.57
1:D:117:ALA:HB1	1:D:148:HIS:NE2	2.19	0.56
1:B:77:ARG:HA	1:B:77:ARG:NE	2.14	0.56
1:B:238:ASP:HA	1:B:242:ARG:HD2	1.88	0.56
1:C:329:ILE:HG13	1:C:330:SER:N	2.20	0.56
1:B:56:GLU:O	1:B:60:VAL:HG23	2.06	0.55
1:D:128:ASP:HB3	4:D:2059:HOH:O	2.05	0.55
1:B:113:ALA:HB2	1:B:141:PRO:HG2	1.89	0.55
1:B:193:GLY:HA3	1:B:200:VAL:HG23	1.89	0.54
1:C:194:GLU:OE1	1:C:321:LYS:NZ	2.38	0.53
1:B:188:GLU:HG2	4:B:2068:HOH:O	2.08	0.53
1:A:66:THR:HG22	1:A:78:VAL:HG21	1.89	0.53
1:D:233:GLN:NE2	4:D:2117:HOH:O	2.42	0.53
1:C:172:PHE:HB2	1:C:191:ILE:HD12	1.91	0.53
1:D:233:GLN:OE1	1:D:237:MET:HE3	2.10	0.52
1:C:109:ARG:HD3	4:C:2091:HOH:O	2.08	0.52
1:B:125:SER:HB3	4:B:2056:HOH:O	2.09	0.51
1:A:306:ASP:HB2	2:A:1001:CL:CL	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:THR:O	3:C:3003:NAD:H2N	2.10	0.50
1:D:291:VAL:HG13	1:D:298:VAL:HG13	1.94	0.50
1:B:117:ALA:N	1:B:118:PRO:HD2	2.26	0.50
1:D:66:THR:O	1:D:70:ILE:HG23	2.11	0.50
1:D:159:GLN:NE2	4:D:2064:HOH:O	2.40	0.50
1:A:193:GLY:HA3	1:A:200:VAL:HG23	1.94	0.50
1:B:188:GLU:HB2	1:B:207:SER:OG	2.12	0.50
1:D:86:GLU:CD	1:D:86:GLU:H	2.20	0.50
1:B:242:ARG:HH11	1:B:242:ARG:HG3	1.78	0.49
1:A:203:PHE:CD2	1:A:225:LYS:HD3	2.48	0.49
1:A:41:ALA:HB1	1:A:70:ILE:HD13	1.96	0.48
1:B:238:ASP:O	1:B:242:ARG:HB2	2.14	0.48
1:B:243:LYS:HZ3	1:B:247:GLU:HB3	1.79	0.48
1:D:225:LYS:O	1:D:229:LEU:HG	2.14	0.47
1:B:275:LEU:HD22	1:B:278:GLU:HB2	1.95	0.47
1:A:110:ILE:HD12	1:A:111:ASP:N	2.29	0.47
1:A:117:ALA:N	1:A:118:PRO:HD2	2.29	0.47
1:D:110:ILE:HD11	1:D:329:ILE:HG23	1.96	0.46
1:D:232:LEU:HD11	4:D:2096:HOH:O	2.15	0.46
1:C:195:HIS:O	1:C:195:HIS:CG	2.68	0.46
1:B:55:LYS:NZ	4:B:2019:HOH:O	2.25	0.46
1:B:269:LEU:O	1:B:291:VAL:HG22	2.17	0.45
1:C:329:ILE:O	1:C:330:SER:C	2.60	0.45
1:B:172:PHE:HB2	1:B:191:ILE:HD12	1.98	0.45
1:B:86:GLU:H	1:B:86:GLU:CD	2.23	0.45
1:C:242:ARG:CZ	4:C:2121:HOH:O	2.65	0.45
1:B:151:GLU:OE2	1:B:274:LYS:HE3	2.16	0.44
1:C:32:VAL:HB	4:C:2065:HOH:O	2.17	0.44
1:D:80:GLN:HE21	1:D:80:GLN:HB3	1.61	0.44
2:A:1005:CL:CL	1:B:73:ASP:OD2	2.73	0.43
1:C:73:ASP:OD2	2:D:1008:CL:CL	2.73	0.43
1:A:138:THR:O	3:A:3001:NAD:H2N	2.17	0.43
1:C:321:LYS:O	1:C:325:GLN:HG3	2.18	0.43
1:A:61:GLY:HA3	1:B:243:LYS:HB2	2.01	0.43
1:C:67:ASN:HD21	1:C:78:VAL:H	1.67	0.43
1:B:275:LEU:HA	1:B:275:LEU:HD23	1.85	0.42
1:A:79:ARG:NH2	4:A:2028:HOH:O	2.52	0.42
1:A:280:GLY:O	4:A:2128:HOH:O	2.21	0.42
1:B:246:THR:HG22	1:B:250:PRO:HD3	2.00	0.42
1:B:142:VAL:HG11	1:B:163:PHE:O	2.19	0.42
1:A:66:THR:CG2	1:A:78:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD22	1:A:163:PHE:HB2	2.02	0.42
1:A:289:VAL:HB	1:A:290:PRO:CD	2.50	0.41
1:A:313:ASP:OD1	4:A:2145:HOH:O	2.21	0.41
1:B:167:LEU:O	1:B:171:ARG:HG3	2.21	0.41
1:B:23:LYS:HE3	1:B:50:VAL:HG21	2.03	0.41
1:B:227:GLN:HB3	4:B:2103:HOH:O	2.20	0.41
1:C:90:GLY:H	1:C:131:ASN:ND2	2.19	0.41
1:C:57:ASP:O	1:D:242:ARG:HB3	2.21	0.41
1:C:91:SER:H	1:C:131:ASN:ND2	2.18	0.41
1:D:241:GLU:OE1	4:D:2121:HOH:O	2.22	0.41
1:A:141:PRO:HB2	4:A:2057:HOH:O	2.20	0.41
1:C:121:GLU:OE2	1:C:148:HIS:NE2	2.47	0.41
1:A:86:GLU:HG2	4:A:2051:HOH:O	2.21	0.40
1:B:23:LYS:HB3	1:B:91:SER:HA	2.04	0.40
1:A:248:TRP:HB3	1:B:38:TYR:CE1	2.56	0.40
1:B:156:SER:H	1:B:159:GLN:HE21	1.69	0.40
1:C:238:ASP:OD1	1:C:242:ARG:NH1	2.53	0.40
1:D:268:VAL:HA	1:D:291:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	248/244 (102%)	236 (95%)	12 (5%)	23	12
1	B	241/244 (99%)	228 (95%)	13 (5%)	20	9
1	C	246/244 (101%)	231 (94%)	15 (6%)	17	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	240/244 (98%)	230 (96%)	10 (4%)	26	16
All	All	975/976 (100%)	925 (95%)	50 (5%)	21	10

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLU
1	A	110	ILE
1	A	132(A)	ASP
1	A	132(B)	ASP
1	A	136	LEU
1	A	142	VAL
1	A	156	SER
1	A	188	GLU
1	A	197	ASP
1	A	200	VAL
1	A	327	ASP
1	A	328	LYS
1	B	70	ILE
1	B	77	ARG
1	B	80	GLN
1	B	86	GLU
1	B	100	ILE
1	B	107	GLN
1	B	109	ARG
1	B	142	VAL
1	B	145	LEU
1	B	197	ASP
1	B	226	GLU
1	B	228	LEU
1	B	301	GLU
1	C	39	ASN
1	C	55	LYS
1	C	109	ARG
1	C	140	ASN
1	C	142	VAL
1	C	156	SER
1	C	191	ILE
1	C	197	ASP
1	C	226	GLU
1	C	234	GLU
1	C	273	VAL

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Mol	Chain	Res	Type
1	C	301	GLU
1	C	310	TYR
1	C	329	ILE
1	C	330	SER
1	D	22	THR
1	D	57	ASP
1	D	86	GLU
1	D	109	ARG
1	D	115	ASP
1	D	122	ASP
1	D	142	VAL
1	D	234	GLU
1	D	301	GLU
1	D	330	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	62	GLN
1	A	80	GLN
1	A	185	GLN
1	A	199	GLN
1	A	233	GLN
1	B	39	ASN
1	B	80	GLN
1	B	107	GLN
1	B	148	HIS
1	B	312	GLN
1	C	39	ASN
1	C	67	ASN
1	C	80	GLN
1	C	131	ASN
1	C	140	ASN
1	C	185	GLN
1	C	199	GLN
1	C	296	ASN
1	C	325	GLN
1	D	67	ASN
1	D	80	GLN
1	D	159	GLN
1	D	227	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAD	A	3001	-	46,48,48	2.15	11 (23%)	64,73,73	1.89	15 (23%)
3	NAD	D	3004	-	46,48,48	1.85	7 (15%)	64,73,73	2.46	25 (39%)
3	NAD	C	3003	-	46,48,48	1.83	7 (15%)	64,73,73	1.96	16 (25%)
3	NAD	B	3002	-	46,48,48	1.97	15 (32%)	64,73,73	2.43	22 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	3001	-	-	5/30/62/62	0/5/5/5
3	NAD	D	3004	-	-	5/30/62/62	0/5/5/5
3	NAD	C	3003	-	-	6/30/62/62	0/5/5/5
3	NAD	B	3002	-	-	3/30/62/62	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3004	NAD	O7N-C7N	7.89	1.38	1.24
3	A	3001	NAD	PA-O3	6.30	1.66	1.59
3	A	3001	NAD	C2N-N1N	5.94	1.41	1.35
3	B	3002	NAD	O7N-C7N	5.76	1.34	1.24
3	D	3004	NAD	O4D-C1D	5.71	1.48	1.40
3	C	3003	NAD	O7N-C7N	5.67	1.34	1.24
3	A	3001	NAD	O7N-C7N	5.51	1.34	1.24
3	C	3003	NAD	C2A-N3A	4.86	1.42	1.33
3	C	3003	NAD	C8A-N7A	4.07	1.39	1.31
3	A	3001	NAD	C5N-C4N	3.79	1.45	1.38
3	C	3003	NAD	C2A-N1A	3.74	1.40	1.33
3	B	3002	NAD	O4D-C1D	3.66	1.45	1.40
3	C	3003	NAD	C5A-N7A	-3.66	1.32	1.39
3	B	3002	NAD	C2A-N3A	3.65	1.40	1.33
3	A	3001	NAD	C8A-N7A	3.50	1.38	1.31
3	B	3002	NAD	C5A-N7A	-3.40	1.32	1.39
3	A	3001	NAD	C5A-N7A	-3.36	1.32	1.39
3	B	3002	NAD	O2D-C2D	-3.31	1.34	1.43
3	B	3002	NAD	C2N-C3N	-3.20	1.33	1.39
3	B	3002	NAD	C8A-N7A	3.18	1.37	1.31
3	C	3003	NAD	C3N-C7N	-3.10	1.46	1.50
3	A	3001	NAD	C3N-C7N	-3.09	1.46	1.50
3	A	3001	NAD	C4N-C3N	2.99	1.43	1.39
3	C	3003	NAD	O3D-C3D	-2.70	1.36	1.43
3	B	3002	NAD	C5A-C4A	-2.65	1.34	1.39
3	A	3001	NAD	C2A-N3A	2.60	1.38	1.33
3	D	3004	NAD	O4B-C1B	-2.58	1.36	1.42
3	D	3004	NAD	C2A-N3A	2.48	1.38	1.33
3	B	3002	NAD	C5D-C4D	2.47	1.59	1.51
3	B	3002	NAD	O3D-C3D	-2.45	1.36	1.43
3	D	3004	NAD	PA-O3	2.27	1.62	1.59
3	B	3002	NAD	PA-O1A	-2.26	1.43	1.50
3	D	3004	NAD	C8A-N7A	2.22	1.35	1.31
3	A	3001	NAD	O4D-C1D	2.21	1.43	1.40
3	A	3001	NAD	C7N-N7N	-2.14	1.29	1.33
3	B	3002	NAD	C6A-N6A	-2.13	1.28	1.34
3	B	3002	NAD	C6N-N1N	2.12	1.40	1.35
3	B	3002	NAD	C7N-N7N	2.11	1.36	1.33
3	D	3004	NAD	C3N-C7N	-2.11	1.47	1.50
3	B	3002	NAD	PA-O2A	-2.02	1.46	1.55

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	NAD	C5A-C4A-N3A	-7.68	116.14	126.72
3	D	3004	NAD	O7N-C7N-N7N	-6.83	112.75	122.62
3	D	3004	NAD	N3A-C2A-N1A	-6.14	119.29	128.58
3	A	3001	NAD	C4D-O4D-C1D	-5.87	104.55	109.92
3	B	3002	NAD	C4D-O4D-C1D	-5.85	104.57	109.92
3	D	3004	NAD	O7N-C7N-C3N	5.67	126.53	119.60
3	B	3002	NAD	C2A-N3A-C4A	5.57	125.44	111.83
3	A	3001	NAD	N3A-C2A-N1A	-5.46	120.31	128.58
3	A	3001	NAD	C3N-C7N-N7N	5.25	124.21	117.74
3	B	3002	NAD	N3A-C2A-N1A	-5.23	120.66	128.58
3	B	3002	NAD	C5A-C4A-N9A	5.13	111.40	105.81
3	D	3004	NAD	N9A-C8A-N7A	-5.07	106.75	113.94
3	C	3003	NAD	C5A-C4A-N3A	-5.05	119.77	126.72
3	D	3004	NAD	C6N-N1N-C2N	-4.90	117.71	121.88
3	C	3003	NAD	C6A-C5A-C4A	4.74	123.65	117.18
3	C	3003	NAD	C4D-O4D-C1D	-4.54	105.77	109.92
3	C	3003	NAD	C5A-C4A-N9A	4.35	110.55	105.81
3	A	3001	NAD	O7N-C7N-N7N	-4.33	116.36	122.62
3	D	3004	NAD	C5A-C4A-N3A	-4.27	120.84	126.72
3	D	3004	NAD	O3D-C3D-C4D	-4.12	99.25	111.08
3	B	3002	NAD	C2A-N1A-C6A	-4.06	112.06	118.73
3	D	3004	NAD	O4B-C1B-N9A	4.04	115.84	108.09
3	C	3003	NAD	N9A-C8A-N7A	-3.98	108.29	113.94
3	B	3002	NAD	C5A-C6A-N1A	3.69	126.87	117.51
3	D	3004	NAD	C5N-C4N-C3N	-3.68	116.75	120.36
3	C	3003	NAD	C5N-C4N-C3N	-3.55	116.88	120.36
3	A	3001	NAD	C5A-C4A-N3A	-3.52	121.86	126.72
3	B	3002	NAD	C5A-N7A-C8A	3.50	108.95	103.45
3	D	3004	NAD	C2N-C3N-C4N	3.40	122.21	118.26
3	A	3001	NAD	O2B-C2B-C1B	3.37	121.72	110.10
3	B	3002	NAD	O2B-C2B-C1B	3.29	121.43	110.10
3	C	3003	NAD	C4A-C5A-N7A	-3.27	106.85	110.58
3	C	3003	NAD	C5A-N7A-C8A	3.24	108.55	103.45
3	D	3004	NAD	C5A-N7A-C8A	3.20	108.49	103.45
3	B	3002	NAD	N9A-C8A-N7A	-3.20	109.40	113.94
3	B	3002	NAD	N3A-C4A-N9A	3.10	132.44	127.17
3	D	3004	NAD	O2N-PN-O1N	3.05	126.66	112.44
3	B	3002	NAD	O4B-C1B-N9A	3.05	113.95	108.09
3	D	3004	NAD	C4A-N9A-C8A	3.04	108.93	105.74
3	C	3003	NAD	C2N-C3N-C4N	3.03	121.78	118.26
3	C	3003	NAD	N3A-C2A-N1A	-3.00	124.04	128.58
3	C	3003	NAD	O2A-PA-O3	3.00	115.37	107.27
3	A	3001	NAD	N9A-C8A-N7A	-2.95	109.74	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3004	NAD	O3B-C3B-C4B	-2.92	102.68	111.08
3	D	3004	NAD	C2A-N1A-C6A	2.88	123.46	118.73
3	C	3003	NAD	O2B-C2B-C1B	2.87	119.98	110.10
3	B	3002	NAD	O7N-C7N-N7N	-2.87	118.47	122.62
3	B	3002	NAD	C4A-C5A-N7A	-2.81	107.36	110.58
3	B	3002	NAD	O2N-PN-O1N	2.78	125.40	112.44
3	A	3001	NAD	C2B-C3B-C4B	2.76	107.94	102.61
3	B	3002	NAD	C4A-N9A-C8A	-2.73	102.87	105.74
3	B	3002	NAD	O2N-PN-O3	2.71	114.60	107.27
3	D	3004	NAD	N3A-C4A-N9A	2.70	131.76	127.17
3	A	3001	NAD	C6N-N1N-C2N	2.69	124.17	121.88
3	B	3002	NAD	O3D-C3D-C4D	-2.68	103.39	111.08
3	D	3004	NAD	C6N-N1N-C1D	2.68	124.98	119.73
3	D	3004	NAD	C2A-N3A-C4A	2.62	118.22	111.83
3	C	3003	NAD	O2N-PN-O1N	2.59	124.50	112.44
3	B	3002	NAD	O7N-C7N-C3N	2.57	122.75	119.60
3	C	3003	NAD	C2B-C3B-C4B	2.57	107.58	102.61
3	A	3001	NAD	O2N-PN-O1N	2.57	124.39	112.44
3	A	3001	NAD	C2A-N3A-C4A	2.51	117.96	111.83
3	B	3002	NAD	N6A-C6A-N1A	-2.44	112.95	118.38
3	D	3004	NAD	O2N-PN-O3	2.43	113.83	107.27
3	D	3004	NAD	O4B-C1B-C2B	2.42	111.80	106.62
3	A	3001	NAD	C3B-C2B-C1B	-2.38	96.97	101.46
3	D	3004	NAD	C5N-C6N-N1N	2.37	123.62	120.38
3	D	3004	NAD	C3N-C7N-N7N	2.37	120.65	117.74
3	D	3004	NAD	C2D-C3D-C4D	2.35	107.14	102.61
3	D	3004	NAD	O3-PN-O1N	-2.29	103.82	110.70
3	C	3003	NAD	C2B-C1B-N9A	-2.25	107.71	113.30
3	A	3001	NAD	C2D-C3D-C4D	2.25	106.95	102.61
3	B	3002	NAD	O4D-C4D-C3D	2.22	109.57	105.15
3	A	3001	NAD	N3A-C4A-N9A	2.13	130.79	127.17
3	B	3002	NAD	C2B-C3B-C4B	2.08	106.63	102.61
3	C	3003	NAD	O3B-C3B-C4B	-2.04	105.22	111.08
3	D	3004	NAD	C2B-C3B-C4B	2.04	106.55	102.61
3	A	3001	NAD	O2A-PA-O3	2.01	112.71	107.27

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	NAD	O4D-C1D-N1N-C2N
3	A	3001	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	A	3001	NAD	C2D-C1D-N1N-C2N
3	A	3001	NAD	C2D-C1D-N1N-C6N
3	B	3002	NAD	O4D-C1D-N1N-C2N
3	B	3002	NAD	O4D-C1D-N1N-C6N
3	B	3002	NAD	C2D-C1D-N1N-C2N
3	C	3003	NAD	O4D-C1D-N1N-C2N
3	C	3003	NAD	O4D-C1D-N1N-C6N
3	C	3003	NAD	C2D-C1D-N1N-C2N
3	D	3004	NAD	O4D-C1D-N1N-C6N
3	D	3004	NAD	O4B-C4B-C5B-O5B
3	C	3003	NAD	O4B-C4B-C5B-O5B
3	C	3003	NAD	C2D-C1D-N1N-C6N
3	D	3004	NAD	C2D-C1D-N1N-C2N
3	D	3004	NAD	C3B-C4B-C5B-O5B
3	D	3004	NAD	O4D-C1D-N1N-C2N
3	A	3001	NAD	O4B-C4B-C5B-O5B
3	C	3003	NAD	C3B-C4B-C5B-O5B

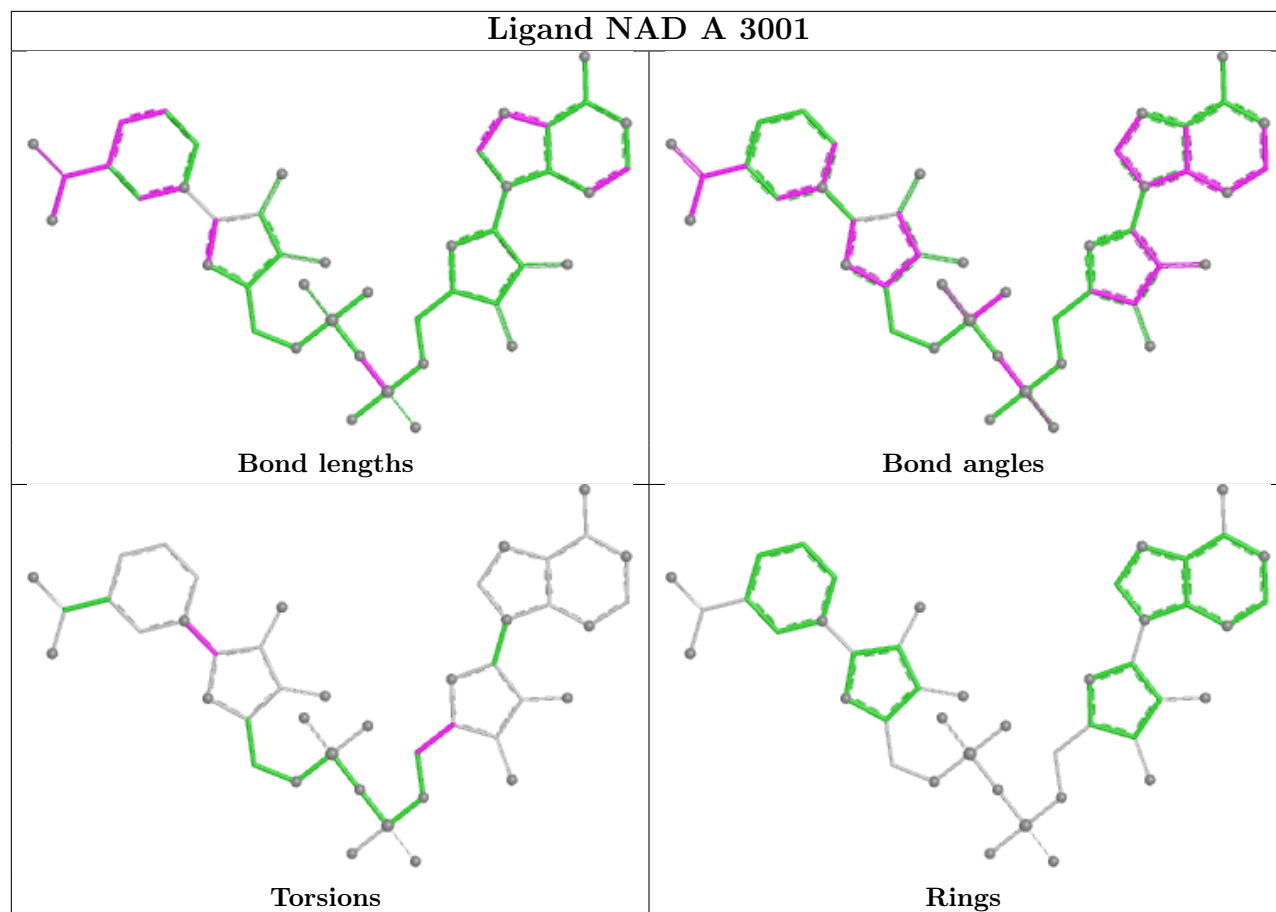
There are no ring outliers.

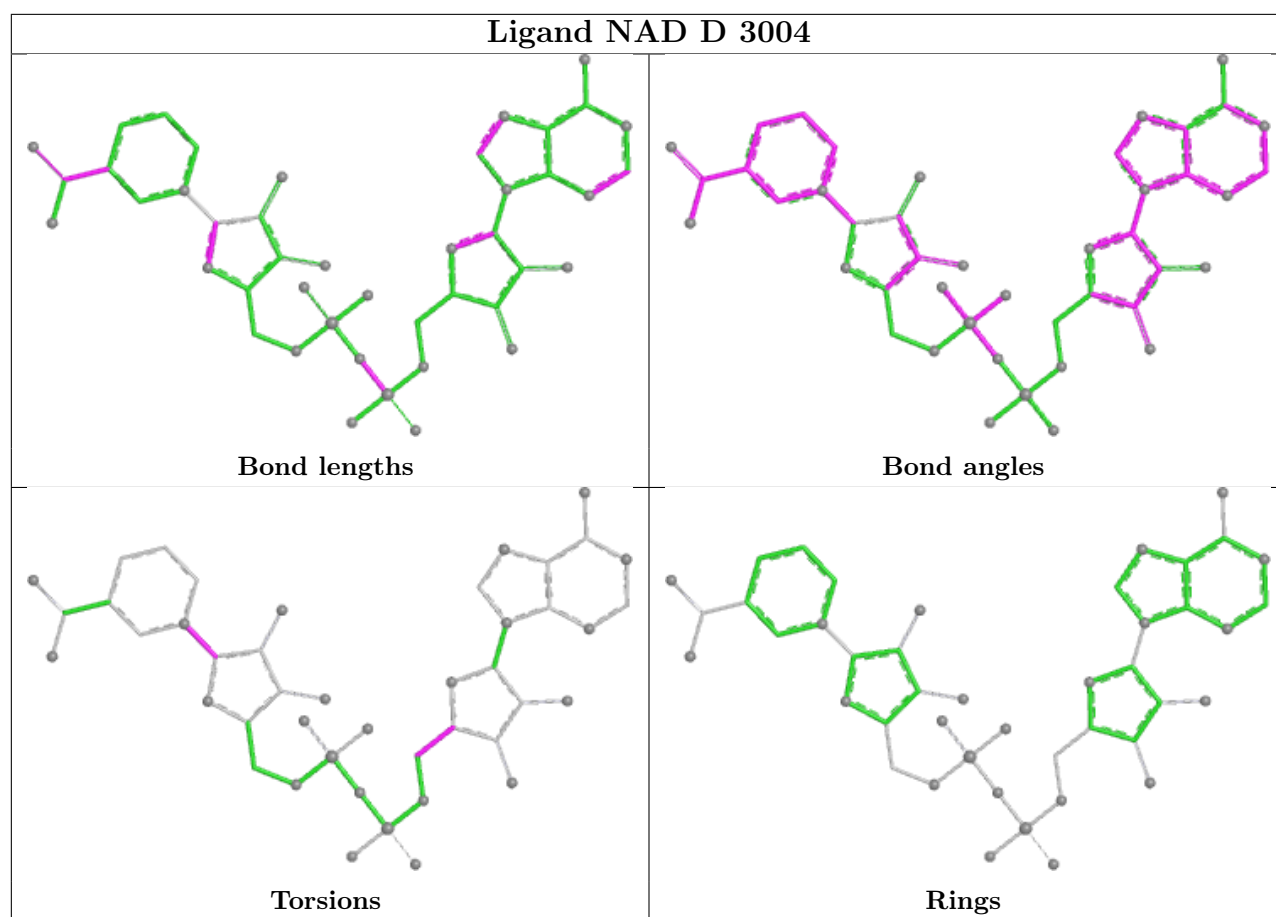
3 monomers are involved in 3 short contacts:

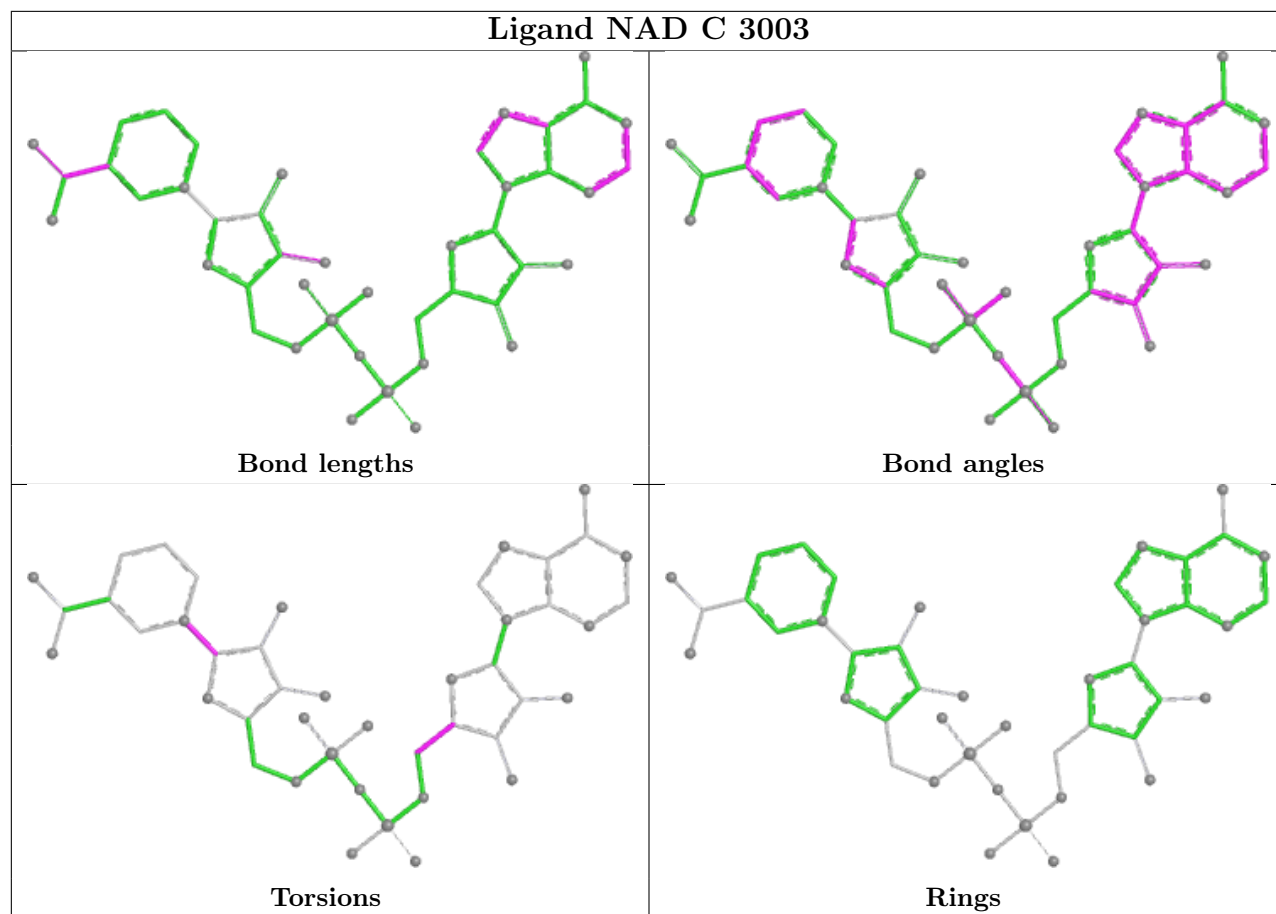
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	NAD	1	0
3	C	3003	NAD	1	0
3	B	3002	NAD	1	0

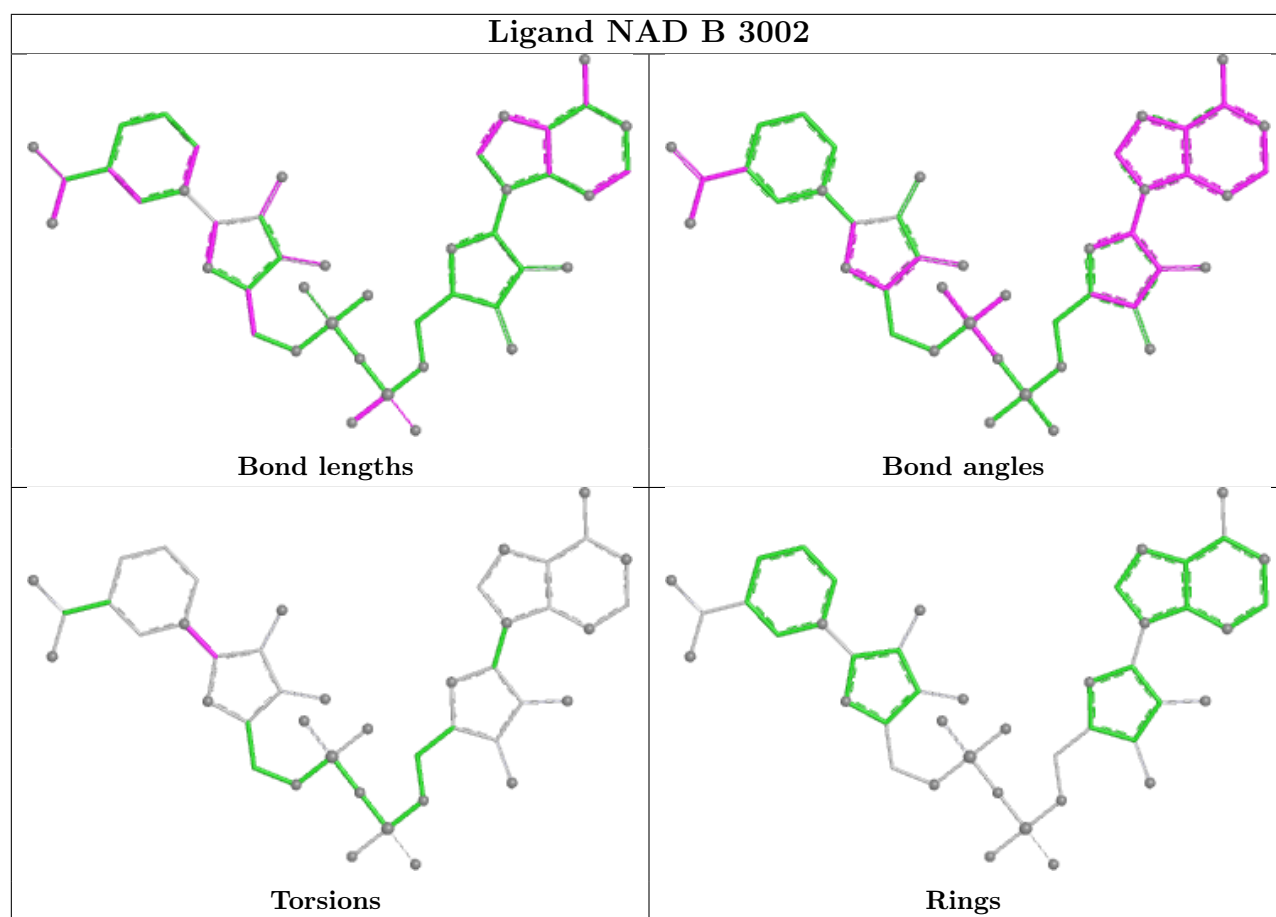
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 3001









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/303 (100%)	-1.00	0 100 100	13, 34, 46, 57	4 (1%)
1	B	298/303 (98%)	-0.95	0 100 100	18, 36, 50, 59	1 (0%)
1	C	303/303 (100%)	-1.03	0 100 100	14, 32, 45, 55	2 (0%)
1	D	298/303 (98%)	-0.97	0 100 100	25, 36, 50, 57	0
All	All	1202/1212 (99%)	-0.99	0 100 100	13, 34, 48, 59	7 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	B	1006	1/1	0.97	0.16	60,60,60,60	0
2	CL	A	1001	1/1	0.99	0.04	36,36,36,36	0
2	CL	C	1007	1/1	0.99	0.08	39,39,39,39	0
2	CL	D	1008	1/1	0.99	0.11	46,46,46,46	0

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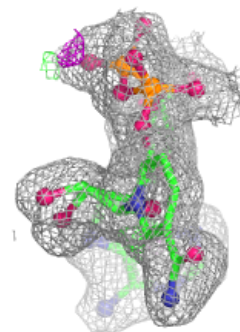
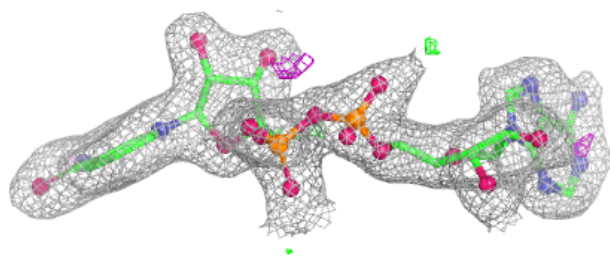
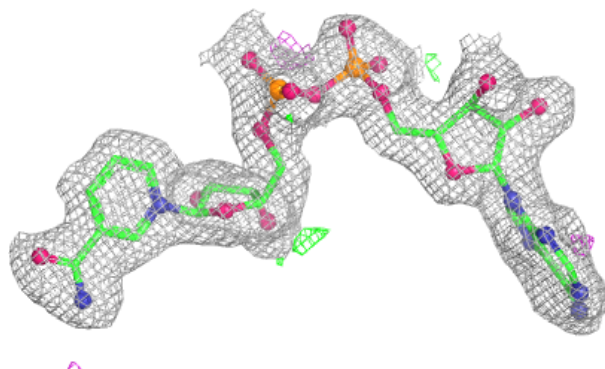
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	A	3001	44/44	0.99	0.03	29,34,40,43	0
3	NAD	B	3002	44/44	0.99	0.04	28,36,42,47	0
3	NAD	C	3003	44/44	0.99	0.03	24,30,38,42	0
3	NAD	D	3004	44/44	0.99	0.04	29,35,43,50	0
2	CL	C	1004	1/1	1.00	0.03	32,32,32,32	0
2	CL	B	1003	1/1	1.00	0.02	36,36,36,36	0
2	CL	D	1002	1/1	1.00	0.04	37,37,37,37	0
2	CL	A	1005	1/1	1.00	0.18	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

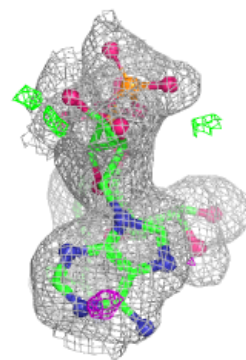
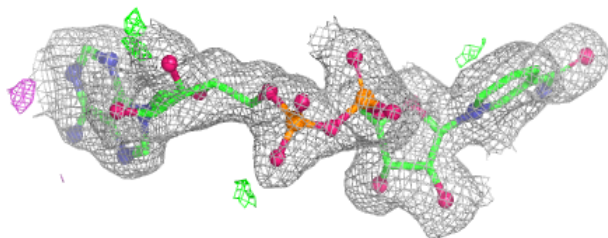
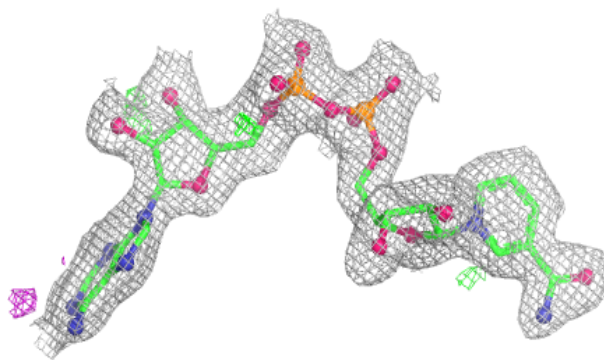
Electron density around NAD A 3001:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

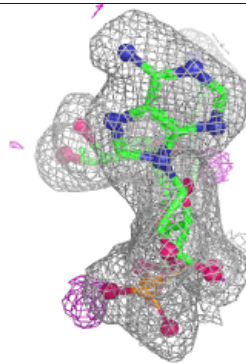
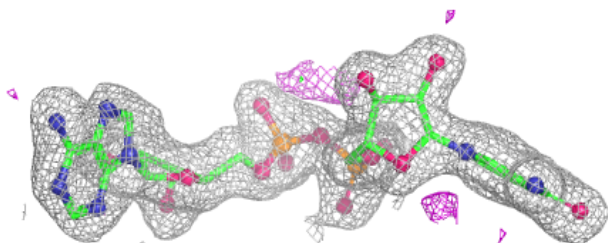
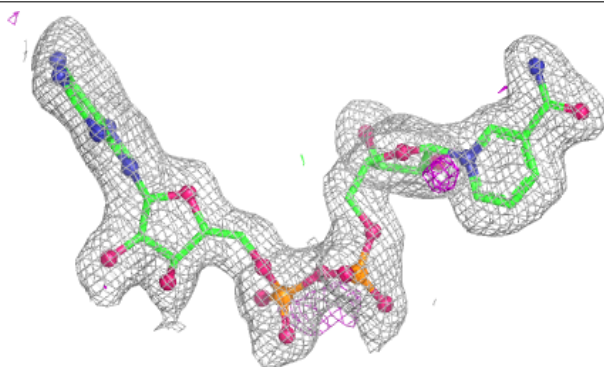


Electron density around NAD B 3002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

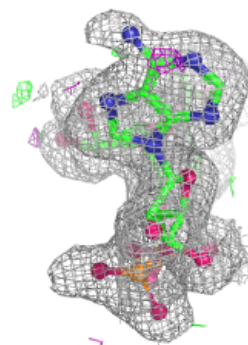
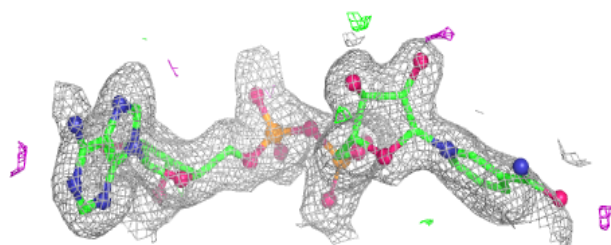
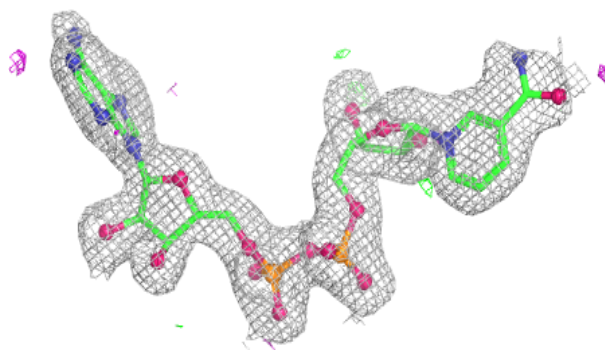
**Electron density around NAD C 3003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD D 3004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.