



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:06 pm BST

PDB ID : 1O6Z
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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

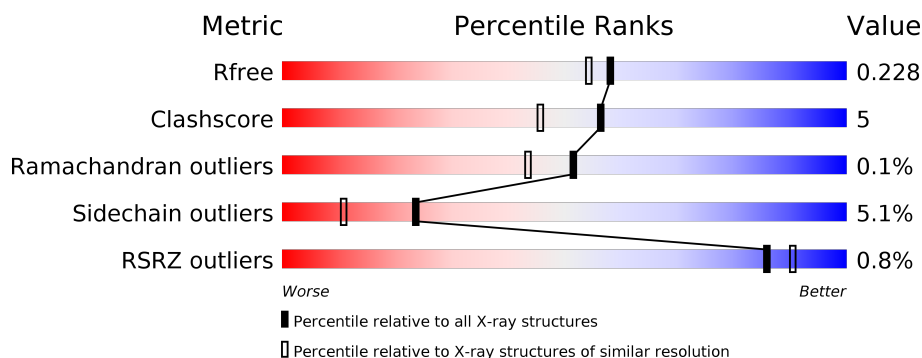
1 Overall quality at a glance

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on 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	<div> <div>2%</div> <div>69% 27% .</div> </div>
1	B	303	<div> <div>67% 27% . .</div> </div>
1	C	303	<div> <div>70% 26% .</div> </div>
1	D	303	<div> <div>2%</div> <div>72% 24% . .</div> </div>

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			

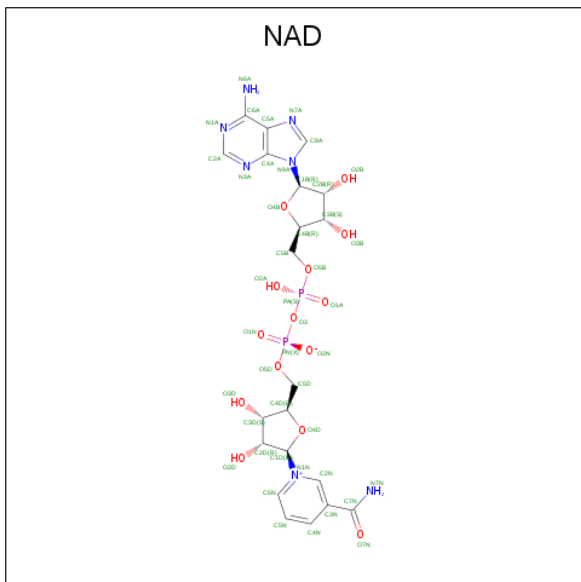
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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

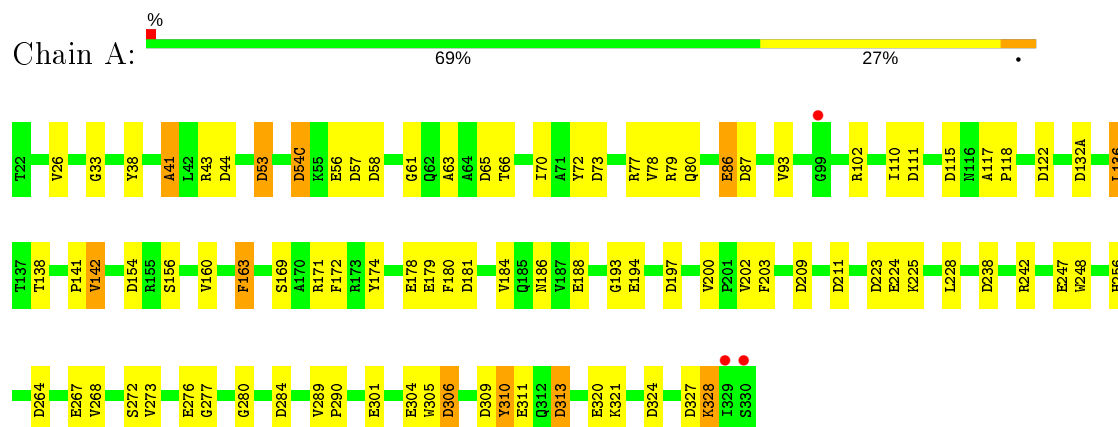
- Molecule 4 is water.

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

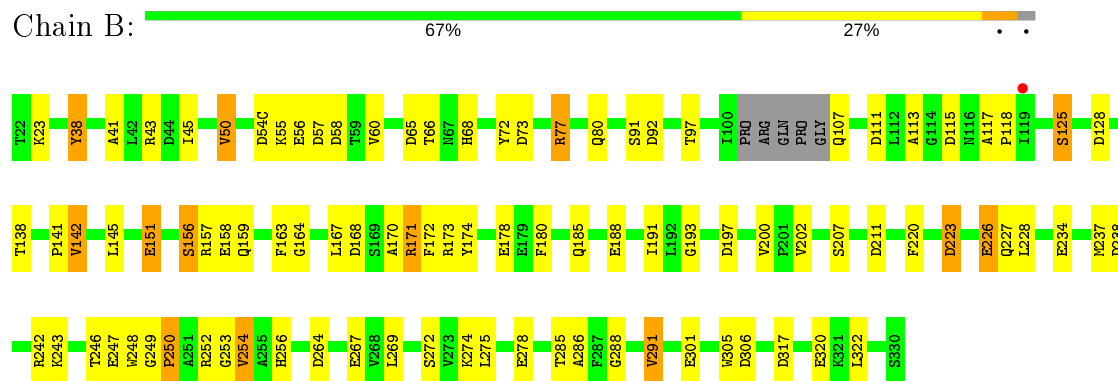
3 Residue-property plots

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

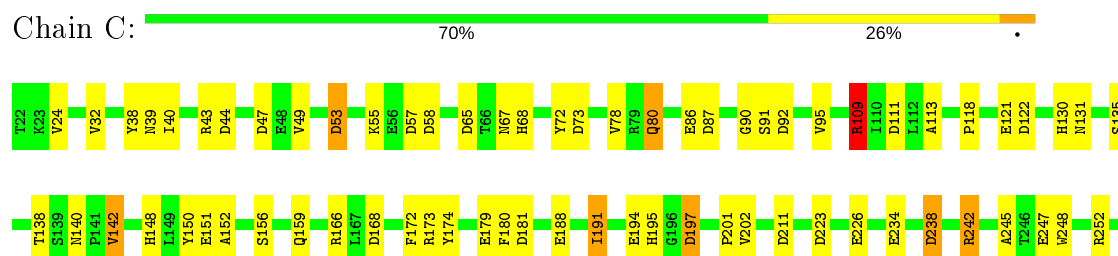
• Molecule 1: MALATE DEHYDROGENASE

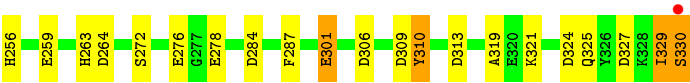


• Molecule 1: MALATE DEHYDROGENASE

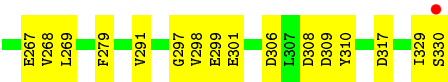


• Molecule 1: MALATE DEHYDROGENASE





● Molecule 1: MALATE DEHYDROGENASE



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 42.42 – 1.96	Depositor EDS
% Data completeness (in resolution range)	78.8 (12.00-1.95) 67.8 (42.42-1.96)	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 0.204 , 0.228	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)	0.33 , 33.2	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	0.91	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: NAD, CL

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	1.81	43/2363 (1.8%)	1.43	32/3210 (1.0%)
1	B	1.85	39/2295 (1.7%)	1.40	22/3116 (0.7%)
1	C	1.84	45/2347 (1.9%)	1.46	38/3188 (1.2%)
1	D	1.83	36/2287 (1.6%)	1.40	29/3105 (0.9%)
All	All	1.83	163/9292 (1.8%)	1.42	121/12619 (1.0%)

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 (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	299	GLU	CD-OE2	-11.32	1.13	1.25
1	B	254	VAL	CB-CG2	-9.40	1.33	1.52
1	A	247	GLU	CD-OE1	8.90	1.35	1.25
1	C	72	TYR	CZ-OH	8.88	1.52	1.37
1	D	234	GLU	CD-OE2	8.76	1.35	1.25
1	A	163	PHE	CE1-CZ	8.64	1.53	1.37
1	C	259	GLU	CD-OE2	8.56	1.35	1.25
1	D	175	VAL	CB-CG1	-8.19	1.35	1.52
1	B	249	GLY	C-O	8.17	1.36	1.23
1	A	178	GLU	CD-OE2	-8.07	1.16	1.25
1	B	170	ALA	CA-CB	-8.05	1.35	1.52
1	D	142	VAL	CB-CG2	-7.88	1.36	1.52
1	C	152	ALA	CA-CB	7.87	1.69	1.52
1	C	38	TYR	CD2-CE2	7.84	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	GLU	CD-OE1	7.55	1.33	1.25
1	C	111	ASP	CB-CG	7.44	1.67	1.51
1	D	27	VAL	CB-CG2	7.36	1.68	1.52
1	B	267	GLU	CD-OE2	7.17	1.33	1.25
1	A	38	TYR	CZ-OH	7.12	1.50	1.37
1	B	158	GLU	CD-OE1	7.11	1.33	1.25
1	A	320	GLU	CD-OE2	7.08	1.33	1.25
1	C	188	GLU	CD-OE1	7.05	1.33	1.25
1	A	72	TYR	CG-CD1	7.04	1.48	1.39
1	D	36	ALA	CA-CB	7.04	1.67	1.52
1	C	324	ASP	CB-CG	6.93	1.66	1.51
1	B	174	TYR	CD2-CE2	-6.90	1.28	1.39
1	A	311	GLU	CD-OE1	6.78	1.33	1.25
1	C	301	GLU	CD-OE2	-6.73	1.18	1.25
1	B	272	SER	CB-OG	6.70	1.50	1.42
1	B	38	TYR	CD1-CE1	-6.68	1.29	1.39
1	C	55	LYS	CB-CG	6.66	1.70	1.52
1	C	272	SER	CB-OG	6.65	1.50	1.42
1	B	291	VAL	CB-CG1	6.64	1.66	1.52
1	D	310	TYR	CE2-CZ	6.63	1.47	1.38
1	A	93	VAL	CB-CG2	6.61	1.66	1.52
1	D	178	GLU	CD-OE2	6.61	1.32	1.25
1	A	256	HIS	C-O	6.58	1.35	1.23
1	D	85	TYR	CD1-CE1	6.55	1.49	1.39
1	B	156	SER	CB-OG	6.55	1.50	1.42
1	D	24	VAL	CB-CG2	6.52	1.66	1.52
1	C	179	GLU	CD-OE2	6.50	1.32	1.25
1	A	180	PHE	CB-CG	-6.46	1.40	1.51
1	C	287	PHE	CB-CG	-6.46	1.40	1.51
1	B	138	THR	CB-CG2	6.43	1.73	1.52
1	C	24	VAL	CB-CG1	6.41	1.66	1.52
1	A	180	PHE	CE2-CZ	-6.40	1.25	1.37
1	A	184	VAL	CB-CG2	6.39	1.66	1.52
1	D	187	VAL	CB-CG1	-6.38	1.39	1.52
1	A	202	VAL	CB-CG1	-6.36	1.39	1.52
1	D	64	ALA	CA-CB	-6.35	1.39	1.52
1	C	306	ASP	CB-CG	6.34	1.65	1.51
1	C	276	GLU	CD-OE2	6.34	1.32	1.25
1	B	174	TYR	CE1-CZ	-6.34	1.30	1.38
1	D	154	ASP	CB-CG	6.32	1.65	1.51
1	D	94	VAL	CB-CG1	-6.31	1.39	1.52
1	C	151	GLU	CD-OE1	6.29	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	VAL	CA-CB	-6.26	1.41	1.54
1	C	40	ILE	C-O	-6.21	1.11	1.23
1	A	163	PHE	CD2-CE2	6.21	1.51	1.39
1	A	163	PHE	CG-CD2	6.21	1.48	1.38
1	C	150	TYR	CE2-CZ	-6.21	1.30	1.38
1	A	310	TYR	CD2-CE2	6.18	1.48	1.39
1	D	204	SER	CB-OG	6.15	1.50	1.42
1	D	310	TYR	CD2-CE2	-6.15	1.30	1.39
1	C	80	GLN	C-O	-6.15	1.11	1.23
1	A	268	VAL	CB-CG1	6.12	1.65	1.52
1	A	267	GLU	CD-OE1	-6.11	1.19	1.25
1	C	86	GLU	CG-CD	6.08	1.61	1.51
1	C	180	PHE	CG-CD1	6.08	1.47	1.38
1	C	188	GLU	CD-OE2	6.06	1.32	1.25
1	B	248	TRP	CZ3-CH2	-6.06	1.30	1.40
1	B	320	GLU	CD-OE2	6.05	1.32	1.25
1	C	174	TYR	CD2-CE2	-6.04	1.30	1.39
1	C	276	GLU	CD-OE1	6.04	1.32	1.25
1	C	68	HIS	C-O	6.04	1.34	1.23
1	A	172	PHE	CE2-CZ	6.04	1.48	1.37
1	D	234	GLU	CD-OE1	5.99	1.32	1.25
1	A	305	TRP	CE3-CZ3	-5.99	1.28	1.38
1	A	273	VAL	CB-CG2	-5.97	1.40	1.52
1	A	228	LEU	C-O	5.97	1.34	1.23
1	A	174	TYR	CD2-CE2	5.96	1.48	1.39
1	D	297	GLY	C-O	5.95	1.33	1.23
1	C	173	ARG	CG-CD	-5.94	1.37	1.51
1	C	49	VAL	CB-CG1	-5.93	1.40	1.52
1	D	279	PHE	CD1-CE1	5.92	1.51	1.39
1	D	38	TYR	CD2-CE2	5.92	1.48	1.39
1	B	41	ALA	CA-CB	5.91	1.64	1.52
1	A	186	ASN	C-O	5.91	1.34	1.23
1	C	310	TYR	CD2-CE2	5.91	1.48	1.39
1	C	248	TRP	CG-CD1	-5.90	1.28	1.36
1	C	113	ALA	CA-CB	-5.89	1.40	1.52
1	D	227	GLN	CG-CD	5.89	1.64	1.51
1	B	185	GLN	CB-CG	5.88	1.68	1.52
1	D	205	LYS	CG-CD	5.88	1.72	1.52
1	B	234	GLU	CD-OE1	5.85	1.32	1.25
1	C	310	TYR	CE2-CZ	5.83	1.46	1.38
1	C	319	ALA	CA-CB	5.83	1.64	1.52
1	D	172	PHE	CE1-CZ	-5.79	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ALA	CA-CB	5.78	1.64	1.52
1	B	68	HIS	C-O	5.78	1.34	1.23
1	D	267	GLU	CD-OE1	5.76	1.31	1.25
1	B	202	VAL	CB-CG2	-5.74	1.40	1.52
1	D	203	PHE	CE2-CZ	5.70	1.48	1.37
1	B	234	GLU	CG-CD	5.69	1.60	1.51
1	C	24	VAL	CA-CB	-5.67	1.42	1.54
1	B	256	HIS	C-O	5.66	1.34	1.23
1	C	263	HIS	C-O	5.65	1.34	1.23
1	B	180	PHE	CE1-CZ	-5.64	1.26	1.37
1	A	171	ARG	CG-CD	5.64	1.66	1.51
1	C	135	SER	CA-CB	5.62	1.61	1.52
1	B	72	TYR	CE1-CZ	5.62	1.45	1.38
1	B	305	TRP	CE2-CZ2	-5.59	1.30	1.39
1	A	56	GLU	CG-CD	5.58	1.60	1.51
1	B	250	PRO	CA-C	-5.54	1.41	1.52
1	B	226	GLU	CD-OE1	5.48	1.31	1.25
1	C	278	GLU	CD-OE1	5.47	1.31	1.25
1	A	93	VAL	CB-CG1	-5.47	1.41	1.52
1	D	237	MET	CG-SD	5.46	1.95	1.81
1	D	86	GLU	CD-OE2	5.46	1.31	1.25
1	A	87	ASP	C-O	5.45	1.33	1.23
1	A	41	ALA	CA-CB	5.45	1.63	1.52
1	B	45	ILE	C-O	5.45	1.33	1.23
1	A	160	VAL	CB-CG1	-5.44	1.41	1.52
1	A	174	TYR	CD1-CE1	5.44	1.47	1.39
1	C	310	TYR	CZ-OH	5.41	1.47	1.37
1	A	180	PHE	CD1-CE1	-5.37	1.28	1.39
1	B	288	GLY	C-O	-5.36	1.15	1.23
1	C	247	GLU	CD-OE1	5.36	1.31	1.25
1	B	267	GLU	CD-OE1	5.36	1.31	1.25
1	A	26	VAL	CA-CB	-5.35	1.43	1.54
1	D	39	ASN	C-O	-5.35	1.13	1.23
1	D	49	VAL	CB-CG1	5.31	1.64	1.52
1	C	256	HIS	C-O	5.30	1.33	1.23
1	B	220	PHE	CE1-CZ	-5.28	1.27	1.37
1	D	308	ASP	CB-CG	-5.27	1.40	1.51
1	A	301	GLU	CD-OE1	5.26	1.31	1.25
1	D	269	LEU	C-O	-5.26	1.13	1.23
1	B	38	TYR	CG-CD1	5.25	1.46	1.39
1	C	159	GLN	C-O	-5.24	1.13	1.23
1	A	277	GLY	C-O	-5.23	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	TYR	CD1-CE1	5.22	1.47	1.39
1	D	188	GLU	CD-OE2	5.22	1.31	1.25
1	D	94	VAL	CB-CG2	5.21	1.63	1.52
1	D	219	GLU	CD-OE1	5.20	1.31	1.25
1	A	224	GLU	CD-OE2	5.19	1.31	1.25
1	A	247	GLU	CG-CD	5.18	1.59	1.51
1	D	258	VAL	CB-CG1	-5.16	1.42	1.52
1	C	118	PRO	CG-CD	5.16	1.67	1.50
1	C	142	VAL	CB-CG1	-5.15	1.42	1.52
1	B	171	ARG	NE-CZ	5.13	1.39	1.33
1	B	253	GLY	N-CA	-5.13	1.38	1.46
1	A	38	TYR	CD2-CE2	-5.12	1.31	1.39
1	C	95	VAL	CB-CG2	5.12	1.63	1.52
1	A	272	SER	CB-OG	5.11	1.48	1.42
1	B	178	GLU	CD-OE2	5.11	1.31	1.25
1	B	291	VAL	C-O	-5.11	1.13	1.23
1	C	202	VAL	CA-CB	-5.10	1.44	1.54
1	B	151	GLU	CG-CD	5.09	1.59	1.51
1	C	72	TYR	CE2-CZ	5.09	1.45	1.38
1	B	285	THR	CA-CB	5.09	1.66	1.53
1	D	51	PHE	CE2-CZ	-5.07	1.27	1.37
1	A	169	SER	C-O	-5.04	1.13	1.23
1	A	33	GLY	C-O	5.03	1.31	1.23

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CB-CG-OD2	11.63	128.77	118.30
1	A	306	ASP	CB-CG-OD2	11.56	128.71	118.30
1	C	181	ASP	CB-CG-OD2	11.40	128.56	118.30
1	C	58	ASP	CB-CG-OD2	10.37	127.64	118.30
1	D	132(B)	ASP	CB-CG-OD2	9.97	127.27	118.30
1	C	87	ASP	CB-CG-OD2	9.91	127.22	118.30
1	D	54(C)	ASP	CB-CG-OD2	9.19	126.57	118.30
1	A	44	ASP	CB-CG-OD2	9.11	126.50	118.30
1	A	54(C)[A]	ASP	CB-CG-OD2	8.79	126.21	118.30
1	A	54(C)[B]	ASP	CB-CG-OD2	8.79	126.21	118.30
1	C	264	ASP	CB-CG-OD1	8.72	126.15	118.30
1	A	211	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	264	ASP	CB-CG-OD2	8.47	125.92	118.30
1	B	65	ASP	CB-CG-OD2	8.45	125.91	118.30
1	D	73	ASP	CB-CG-OD2	8.33	125.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	CB-CG-OD2	8.27	125.74	118.30
1	C	284	ASP	CB-CG-OD1	8.17	125.65	118.30
1	D	211	ASP	CB-CG-OD2	8.02	125.52	118.30
1	B	54(C)	ASP	CB-CG-OD2	8.00	125.50	118.30
1	B	211	ASP	CB-CG-OD1	7.94	125.45	118.30
1	A	154	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	115	ASP	CB-CG-OD2	7.90	125.41	118.30
1	C	43[A]	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	C	43[B]	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	C	53	ASP	CB-CG-OD2	7.76	125.28	118.30
1	C	252	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	C	306	ASP	CB-CG-OD2	7.74	125.27	118.30
1	D	242	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	C	122	ASP	CB-CG-OD1	7.62	125.16	118.30
1	C	223	ASP	CB-CG-OD2	7.20	124.78	118.30
1	D	242	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	173	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	D	58	ASP	CB-CG-OD2	7.04	124.64	118.30
1	B	157	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	309	ASP	CB-CG-OD2	6.95	124.56	118.30
1	B	115	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	109	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	B	252	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	211	ASP	CB-CG-OD2	6.78	124.40	118.30
1	C	168	ASP	CB-CG-OD2	6.77	124.39	118.30
1	C	324	ASP	CB-CG-OD2	6.77	124.39	118.30
1	B	111	ASP	CB-CG-OD2	6.75	124.37	118.30
1	B	223	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	231	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	171	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	C	245	ALA	CB-CA-C	-6.63	100.16	110.10
1	D	115	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	238	ASP	CB-CG-OD2	6.56	124.21	118.30
1	B	306	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	168	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	122[A]	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	122[B]	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	53	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	313	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	77	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	317	ASP	CB-CG-OD2	6.24	123.91	118.30
1	C	65	ASP	CB-CG-OD1	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	309	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	197	ASP	CB-CG-OD2	6.15	123.83	118.30
1	D	306	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	181	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	B	57	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	276	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	65	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	324	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	324	ASP	OD1-CG-OD2	-6.02	111.86	123.30
1	A	304	GLU	OE1-CD-OE2	6.02	130.52	123.30
1	C	201	PRO	N-CD-CG	-6.01	94.19	103.20
1	C	44	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	324	ASP	CB-CG-OD2	5.97	123.67	118.30
1	D	132(B)	ASP	OD1-CG-OD2	-5.95	111.99	123.30
1	C	111	ASP	OD1-CG-OD2	-5.91	112.08	123.30
1	B	174	TYR	CG-CD1-CE1	-5.88	116.59	121.30
1	D	118	PRO	N-CD-CG	-5.87	94.40	103.20
1	D	53	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	168	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	209	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	284	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	313[A]	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	313[B]	ASP	CB-CG-OD2	5.77	123.50	118.30
1	D	171	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	309	ASP	CB-CG-OD2	5.75	123.47	118.30
1	D	46	ALA	N-CA-CB	-5.75	102.05	110.10
1	C	87	ASP	OD1-CG-OD2	-5.71	112.46	123.30
1	D	120	MET	CG-SD-CE	5.70	109.32	100.20
1	C	327	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	97	THR	OG1-CB-CG2	-5.70	96.90	110.00
1	A	58	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	237	MET	CG-SD-CE	5.67	109.27	100.20
1	C	191	ILE	CG1-CB-CG2	-5.64	98.99	111.40
1	C	109	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	313	ASP	OD1-CG-OD2	-5.57	112.71	123.30
1	C	92	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	242	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	B	38	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	87	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	58	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	317	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	22	THR	OG1-CB-CG2	-5.46	97.43	110.00
1	B	264	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	313	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	57	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	66	THR	OG1-CB-CG2	-5.41	97.56	110.00
1	D	223	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	151	GLU	OE1-CD-OE2	-5.31	116.92	123.30
1	A	181[A]	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	181[B]	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	252	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	D	52	VAL	CB-CA-C	-5.18	101.55	111.40
1	C	174	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
1	D	77	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	181	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	48	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	D	234	GLU	OE1-CD-OE2	5.07	129.39	123.30
1	A	223	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	102	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	47	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	179	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	142	VAL	CA-CB-CG2	5.02	118.44	110.90

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 ⓘ

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	32	0
1	C	2310	0	2164	19	0
1	D	2253	0	2110	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	10011	0	8659	90	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 (90) 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:HE	1:B:77:ARG:HA	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: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:NE	1:B:77:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:159:GLN:NE2	4:D:2064:HOH:O	2.40	0.50
1:D:66:THR:O	1:D:70:ILE:HG23	2.11	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:B:242:ARG:HG3	1:B:242:ARG:HH11	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:A:328:LYS:NZ	4:A:2155:HOH:O	2.32	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:B:243:LYS:HZ3	1:B:247:GLU:HB3	1.80	0.46
1:D:232:LEU:HD11	4:D:2096:HOH:O	2.15	0.46
1:C:195:HIS:CG	1:C:195:HIS:O	2.68	0.46
1:B:269:LEU:O	1:B:291:VAL:HG22	2.17	0.45
1:B:172:PHE:HB2	1:B:191:ILE:HD12	1.98	0.45
1:D:86:GLU:CD	1:D:86:GLU:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:GLY:O	4:A:2128:HOH:O	2.21	0.42
1:A:79:ARG:NH2	4:A:2028:HOH:O	2.52	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
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:B:55:LYS:NZ	4:B:2019:HOH:O	2.25	0.41
1:C:121:GLU:OE2	1:C:148:HIS:NE2	2.47	0.41
1:A:141:PRO:HB2	4:A:2057:HOH:O	2.20	0.41
1:C:329:ILE:O	1:C:330:SER:C	2.60	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](#)

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	305/303 (101%)	294 (96%)	11 (4%)	0	100	100
1	B	295/303 (97%)	282 (96%)	12 (4%)	1 (0%)	41	30
1	C	303/303 (100%)	294 (97%)	9 (3%)	0	100	100
1	D	294/303 (97%)	285 (97%)	9 (3%)	0	100	100
All	All	1197/1212 (99%)	1155 (96%)	41 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/244 (102%)	236 (95%)	12 (5%)	25	12
1	B	241/244 (99%)	229 (95%)	12 (5%)	24	11
1	C	246/244 (101%)	232 (94%)	14 (6%)	20	9
1	D	240/244 (98%)	229 (95%)	11 (5%)	27	14
All	All	975/976 (100%)	926 (95%)	49 (5%)	24	11

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	80	GLN
1	A	86	GLU
1	A	132(A)	ASP
1	A	136	LEU
1	A	142	VAL
1	A	156	SER
1	A	188	GLU
1	A	197	ASP
1	A	310	TYR

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Mol	Chain	Res	Type
1	A	327	ASP
1	A	328	LYS
1	B	43	ARG
1	B	77	ARG
1	B	80	GLN
1	B	107	GLN
1	B	125	SER
1	B	142	VAL
1	B	145	LEU
1	B	197	ASP
1	B	223	ASP
1	B	226	GLU
1	B	228	LEU
1	B	301	GLU
1	C	39	ASN
1	C	53	ASP
1	C	80	GLN
1	C	109	ARG
1	C	140	ASN
1	C	142	VAL
1	C	156	SER
1	C	197	ASP
1	C	226	GLU
1	C	234	GLU
1	C	301	GLU
1	C	310	TYR
1	C	329	ILE
1	C	330	SER
1	D	57	ASP
1	D	80	GLN
1	D	86	GLU
1	D	109	ARG
1	D	115	ASP
1	D	122	ASP
1	D	132(B)	ASP
1	D	142	VAL
1	D	234	GLU
1	D	301	GLU
1	D	330	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	62	GLN
1	A	80	GLN
1	A	146	ASN
1	A	199	GLN
1	A	233	GLN
1	B	39	ASN
1	B	80	GLN
1	B	140	ASN
1	B	148	HIS
1	B	159	GLN
1	B	185	GLN
1	C	67	ASN
1	C	80	GLN
1	C	131	ASN
1	C	140	ASN
1	C	325	GLN
1	D	67	ASN
1	D	80	GLN
1	D	131	ASN
1	D	146	ASN
1	D	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	D	3004	-	42,48,48	1.89	5 (11%)	50,73,73	2.35	17 (34%)
3	NAD	C	3003	-	42,48,48	1.93	8 (19%)	50,73,73	1.48	11 (22%)
3	NAD	A	3001	-	42,48,48	1.90	8 (19%)	50,73,73	1.83	11 (22%)
3	NAD	B	3002	-	42,48,48	2.07	12 (28%)	50,73,73	1.77	13 (26%)

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	D	3004	-	-	4/26/62/62	0/5/5/5
3	NAD	C	3003	-	-	6/26/62/62	0/5/5/5
3	NAD	A	3001	-	-	5/26/62/62	0/5/5/5
3	NAD	B	3002	-	-	4/26/62/62	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3004	NAD	O7N-C7N	7.66	1.38	1.24
3	C	3003	NAD	C2A-N3A	6.49	1.42	1.32
3	B	3002	NAD	O7N-C7N	5.59	1.34	1.24
3	C	3003	NAD	O7N-C7N	5.51	1.34	1.24
3	A	3001	NAD	C2N-N1N	5.37	1.41	1.35
3	A	3001	NAD	O7N-C7N	5.35	1.34	1.24
3	D	3004	NAD	O4D-C1D	5.24	1.48	1.41
3	B	3002	NAD	C2A-N3A	5.16	1.40	1.32
3	A	3001	NAD	C2A-N3A	4.00	1.38	1.32
3	D	3004	NAD	C2A-N3A	3.87	1.38	1.32
3	D	3004	NAD	O4B-C1B	-3.61	1.36	1.41
3	C	3003	NAD	C2A-N1A	3.59	1.40	1.33
3	B	3002	NAD	O2D-C2D	-3.49	1.34	1.43
3	B	3002	NAD	O4D-C1D	3.31	1.45	1.41
3	B	3002	NAD	C2N-C3N	-3.27	1.33	1.39
3	B	3002	NAD	C2D-C1D	3.12	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	NAD	C5N-C4N	3.07	1.45	1.38
3	C	3003	NAD	C3N-C7N	-3.06	1.46	1.50
3	A	3001	NAD	C3N-C7N	-3.05	1.46	1.50
3	C	3003	NAD	C4A-N3A	-3.00	1.31	1.35
3	B	3002	NAD	C4A-N3A	-2.88	1.31	1.35
3	C	3003	NAD	O3D-C3D	-2.85	1.36	1.43
3	A	3001	NAD	C4N-C3N	2.72	1.43	1.39
3	C	3003	NAD	C8A-N7A	2.69	1.39	1.34
3	B	3002	NAD	O3D-C3D	-2.58	1.36	1.43
3	B	3002	NAD	C5A-C4A	-2.48	1.34	1.40
3	B	3002	NAD	C5D-C4D	2.37	1.59	1.51
3	B	3002	NAD	PA-O1A	-2.23	1.43	1.50
3	A	3001	NAD	C8A-N7A	2.08	1.38	1.34
3	A	3001	NAD	C7N-N7N	-2.08	1.29	1.33
3	D	3004	NAD	C3N-C7N	-2.07	1.47	1.50
3	B	3002	NAD	C7N-N7N	2.03	1.36	1.33
3	C	3003	NAD	C5A-N7A	-2.02	1.32	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3004	NAD	O7N-C7N-N7N	-6.92	112.75	122.58
3	D	3004	NAD	N3A-C2A-N1A	-6.01	119.29	128.68
3	D	3004	NAD	O7N-C7N-C3N	5.76	126.53	119.63
3	A	3001	NAD	C3N-C7N-N7N	5.38	124.21	117.75
3	A	3001	NAD	N3A-C2A-N1A	-5.35	120.31	128.68
3	B	3002	NAD	N3A-C2A-N1A	-5.13	120.66	128.68
3	D	3004	NAD	C6N-N1N-C2N	-4.68	117.71	121.97
3	A	3001	NAD	O7N-C7N-N7N	-4.38	116.36	122.58
3	D	3004	NAD	O3D-C3D-C4D	-4.08	99.25	111.05
3	B	3002	NAD	C2A-N1A-C6A	-3.91	112.06	118.75
3	D	3004	NAD	C2N-C3N-C4N	3.48	122.21	118.26
3	D	3004	NAD	O4B-C1B-C2B	3.34	111.80	106.93
3	A	3001	NAD	PN-O3-PA	-3.22	121.77	132.83
3	C	3003	NAD	C2N-C3N-C4N	3.11	121.78	118.26
3	D	3004	NAD	C5N-C4N-C3N	-3.03	116.75	120.34
3	C	3003	NAD	N3A-C2A-N1A	-2.96	124.04	128.68
3	A	3001	NAD	O2B-C2B-C1B	2.94	121.72	110.85
3	C	3003	NAD	C5N-C4N-C3N	-2.93	116.88	120.34
3	D	3004	NAD	O2N-PN-O1N	2.92	126.66	112.24
3	D	3004	NAD	O3B-C3B-C4B	-2.89	102.68	111.05
3	B	3002	NAD	O7N-C7N-N7N	-2.89	118.47	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	NAD	C5A-C6A-N1A	2.88	126.87	120.35
3	B	3002	NAD	O2B-C2B-C1B	2.86	121.43	110.85
3	D	3004	NAD	PN-O3-PA	-2.86	123.02	132.83
3	A	3001	NAD	O4D-C1D-C2D	2.77	110.97	106.93
3	D	3004	NAD	C2A-N1A-C6A	2.75	123.46	118.75
3	A	3001	NAD	C2B-C3B-C4B	2.72	107.94	102.64
3	B	3002	NAD	N6A-C6A-N1A	-2.71	112.95	118.57
3	A	3001	NAD	C3B-C2B-C1B	-2.66	96.97	100.98
3	B	3002	NAD	O2N-PN-O1N	2.66	125.40	112.24
3	B	3002	NAD	O3D-C3D-C4D	-2.65	103.39	111.05
3	B	3002	NAD	O7N-C7N-C3N	2.60	122.75	119.63
3	C	3003	NAD	C2B-C3B-C4B	2.54	107.58	102.64
3	C	3003	NAD	O2N-PN-O1N	2.48	124.50	112.24
3	C	3003	NAD	O2B-C2B-C1B	2.47	119.98	110.85
3	A	3001	NAD	O2N-PN-O1N	2.46	124.39	112.24
3	C	3003	NAD	C4A-C5A-N7A	-2.45	106.85	109.40
3	B	3002	NAD	PN-O3-PA	-2.43	124.49	132.83
3	D	3004	NAD	C3N-C7N-N7N	2.42	120.65	117.75
3	A	3001	NAD	C6N-N1N-C2N	2.40	124.17	121.97
3	B	3002	NAD	O4B-C1B-C2B	-2.34	103.50	106.93
3	D	3004	NAD	C2D-C3D-C4D	2.32	107.14	102.64
3	B	3002	NAD	O4D-C4D-C3D	2.25	109.57	105.11
3	D	3004	NAD	C5N-C6N-N1N	2.25	123.62	120.40
3	A	3001	NAD	C2D-C3D-C4D	2.22	106.95	102.64
3	D	3004	NAD	C1B-N9A-C4A	-2.11	122.93	126.64
3	C	3003	NAD	PN-O3-PA	-2.06	125.77	132.83
3	B	3002	NAD	C2B-C3B-C4B	2.05	106.63	102.64
3	C	3003	NAD	O2D-C2D-C1D	2.02	118.32	110.85
3	C	3003	NAD	O3B-C3B-C4B	-2.02	105.22	111.05
3	D	3004	NAD	C2B-C3B-C4B	2.01	106.55	102.64
3	C	3003	NAD	O4D-C1D-C2D	2.00	109.85	106.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3004	NAD	O4D-C1D-N1N-C6N
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	A	3001	NAD	O4D-C1D-N1N-C2N
3	A	3001	NAD	O4D-C1D-N1N-C6N

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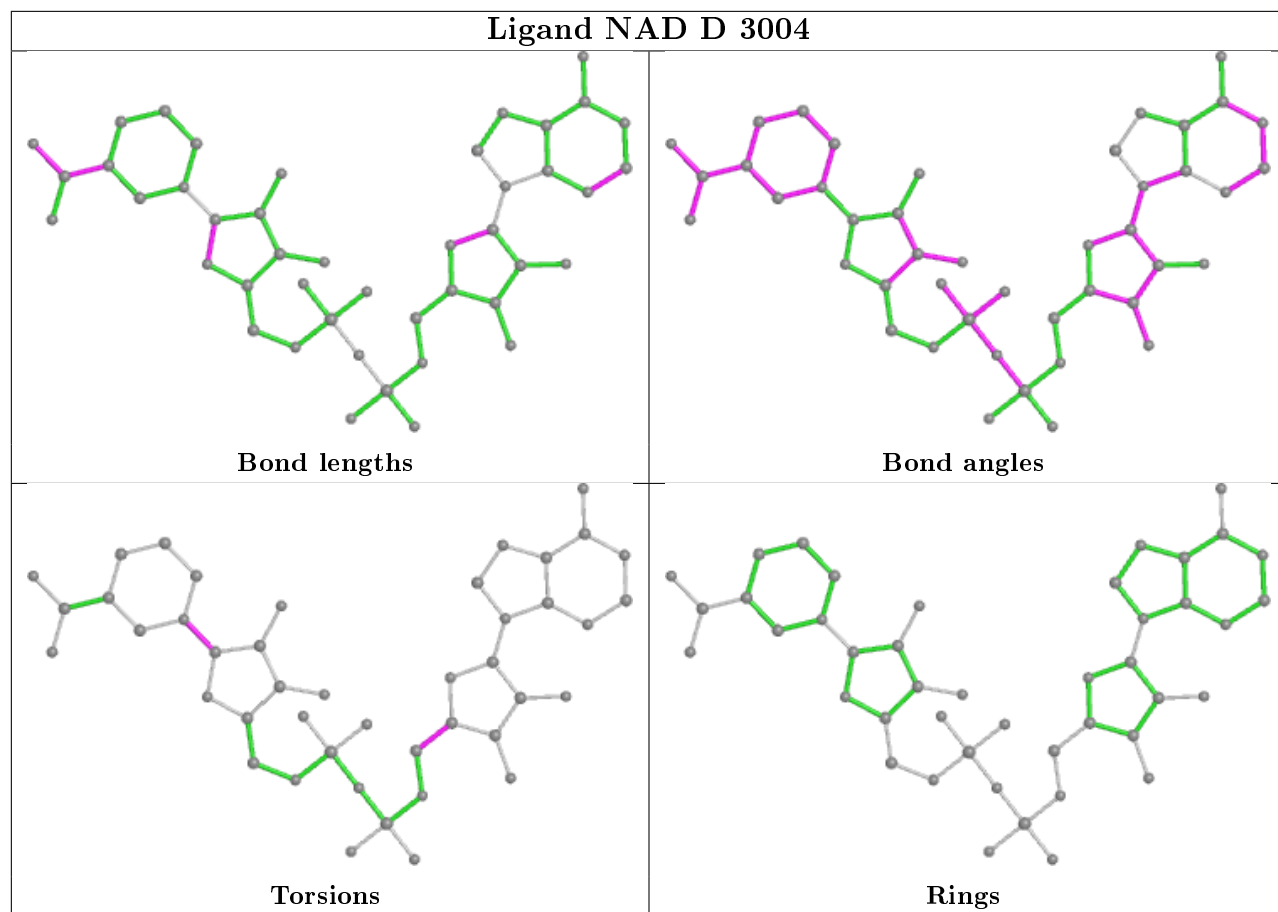
Mol	Chain	Res	Type	Atoms
3	A	3001	NAD	C2D-C1D-N1N-C2N
3	A	3001	NAD	C2D-C1D-N1N-C6N
3	B	3002	NAD	O4D-C1D-N1N-C2N
3	B	3002	NAD	O4D-C1D-N1N-C6N
3	B	3002	NAD	C2D-C1D-N1N-C2N
3	D	3004	NAD	O4B-C4B-C5B-O5B
3	C	3003	NAD	O4B-C4B-C5B-O5B
3	D	3004	NAD	C3B-C4B-C5B-O5B
3	A	3001	NAD	O4B-C4B-C5B-O5B
3	C	3003	NAD	C3B-C4B-C5B-O5B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

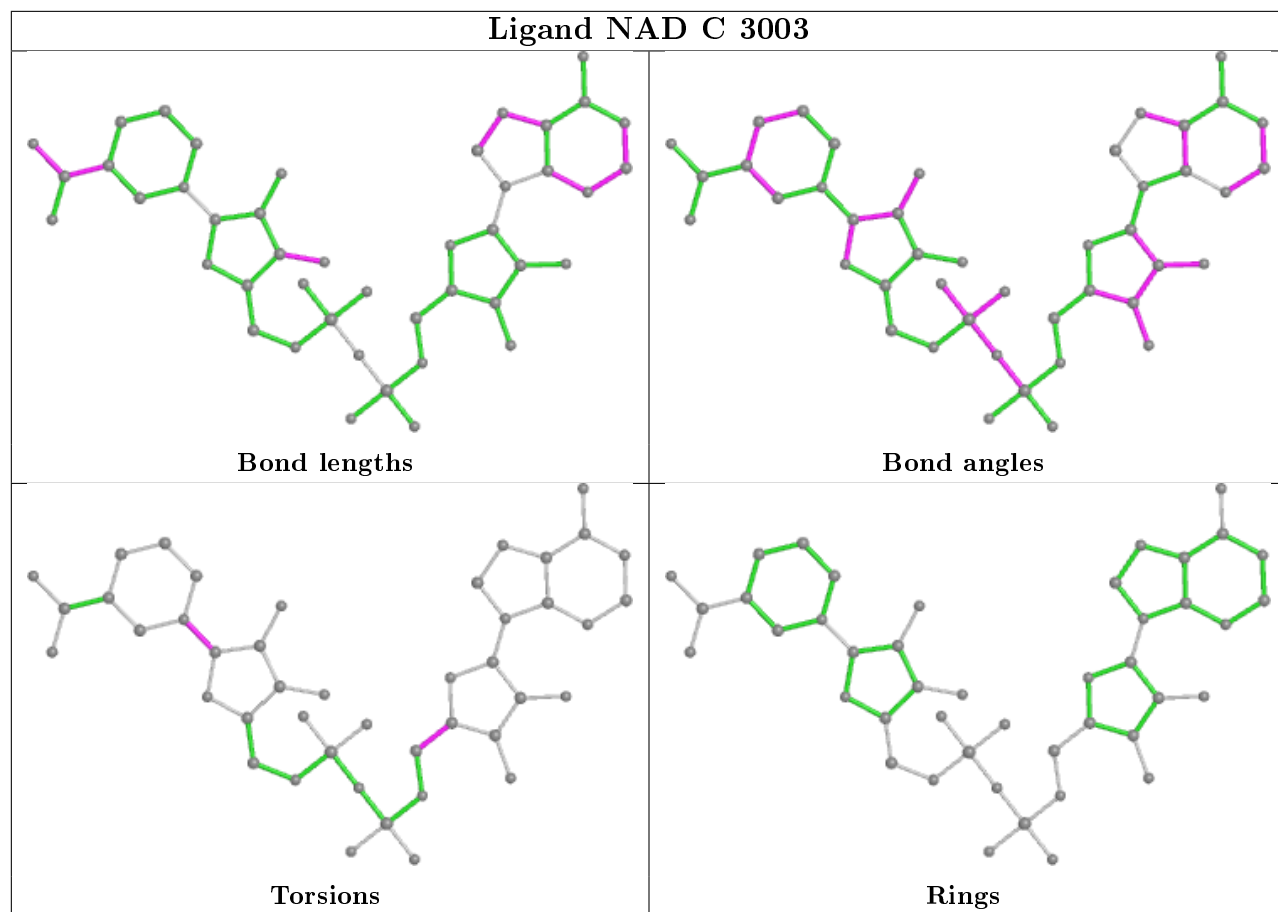
There are no ring outliers.

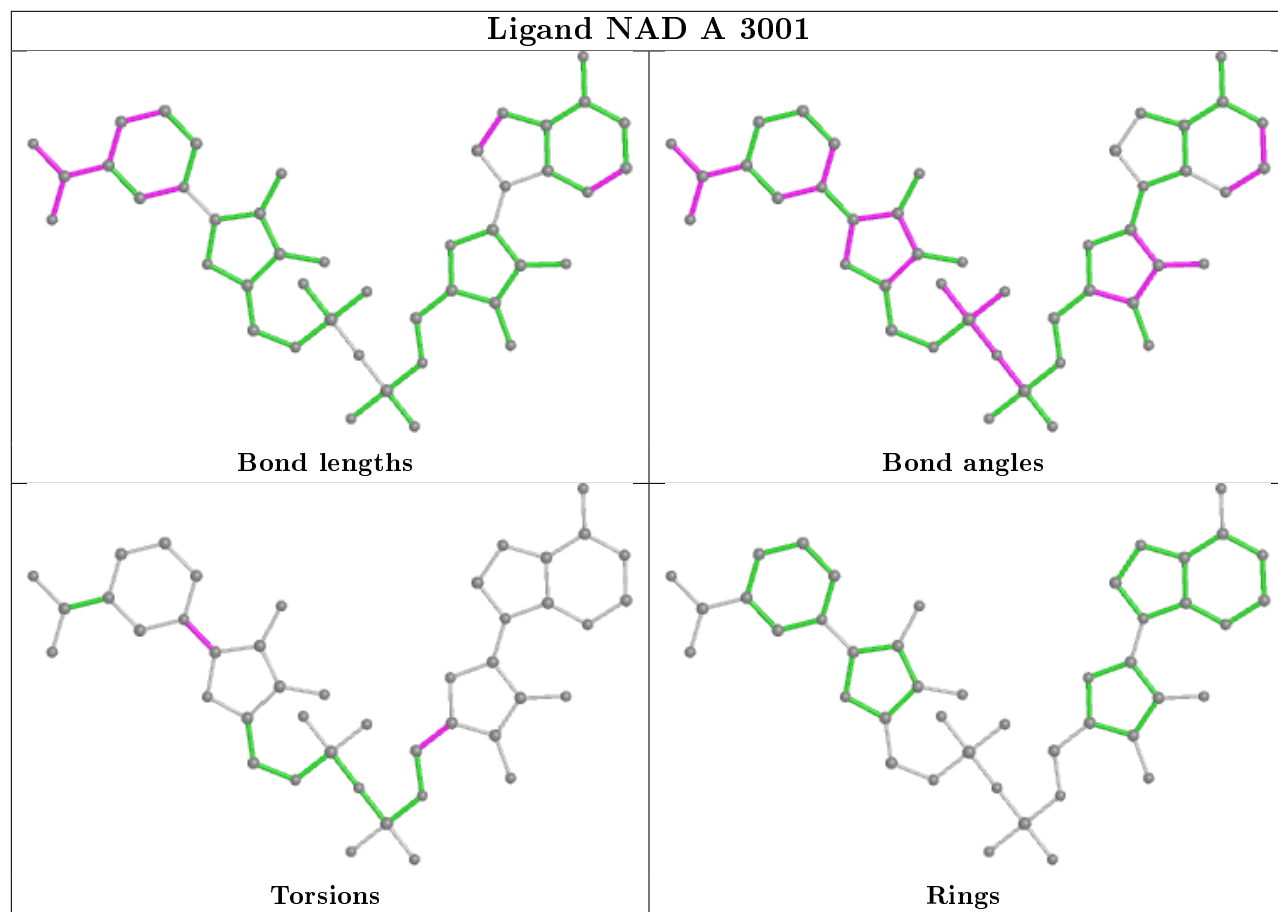
3 monomers are involved in 3 short contacts:

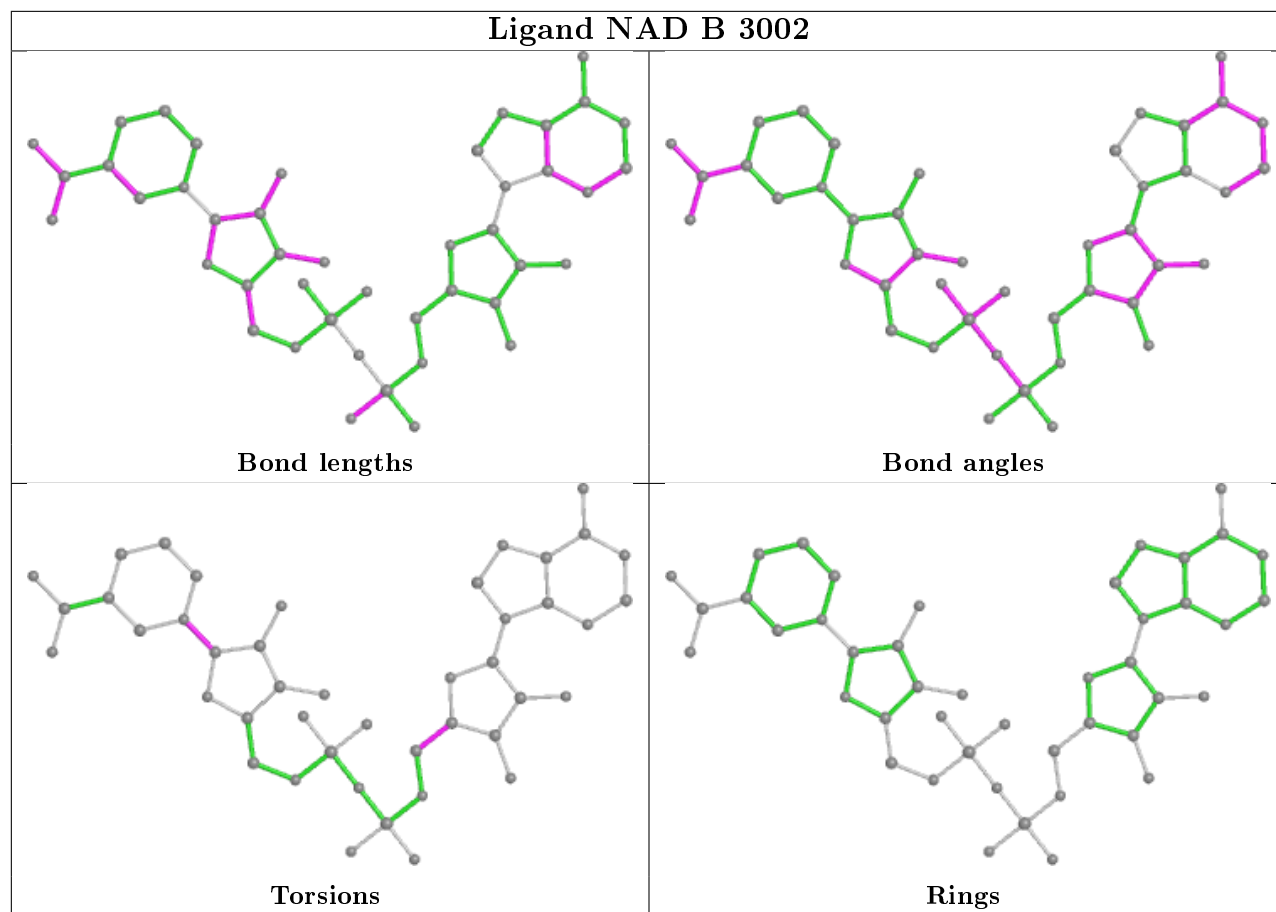
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3003	NAD	1	0
3	A	3001	NAD	1	0
3	B	3002	NAD	1	0

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.









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%)	0.00	3 (0%) 82 87	25, 35, 46, 57	0
1	B	298/303 (98%)	0.05	1 (0%) 94 96	25, 36, 50, 59	0
1	C	303/303 (100%)	-0.05	1 (0%) 94 96	24, 32, 45, 55	0
1	D	298/303 (98%)	0.06	5 (1%) 70 77	25, 36, 50, 57	0
All	All	1202/1212 (99%)	0.02	10 (0%) 86 90	24, 34, 48, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	3.2
1	A	99	GLY	2.6
1	D	330	SER	2.6
1	A	329	ILE	2.6
1	D	154	ASP	2.4
1	D	132(A)	ASP	2.3
1	B	119	ILE	2.1
1	D	227	GLN	2.1
1	D	132(B)	ASP	2.1
1	C	330	SER	2.0

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 carbohydrates in this entry.

6.4 Ligands

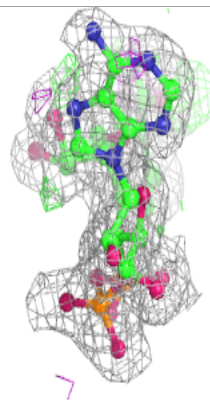
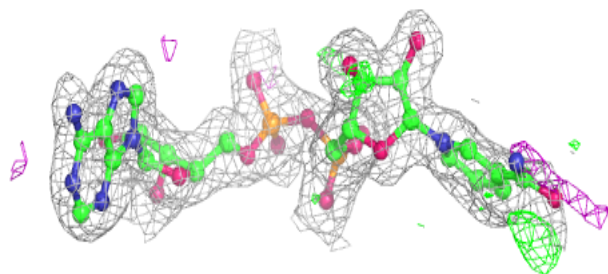
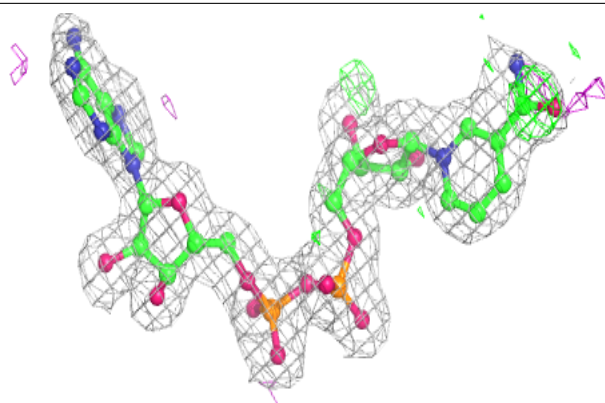
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.88	0.30	60,60,60,60	0
3	NAD	D	3004	44/44	0.94	0.12	29,35,43,50	0
2	CL	D	1002	1/1	0.96	0.05	37,37,37,37	0
3	NAD	C	3003	44/44	0.96	0.11	24,30,38,42	0
3	NAD	A	3001	44/44	0.96	0.10	29,34,40,43	0
3	NAD	B	3002	44/44	0.96	0.11	28,36,42,47	0
2	CL	D	1008	1/1	0.97	0.10	46,46,46,46	0
2	CL	C	1004	1/1	0.97	0.10	32,32,32,32	0
2	CL	C	1007	1/1	0.98	0.08	39,39,39,39	0
2	CL	A	1001	1/1	0.98	0.08	36,36,36,36	0
2	CL	A	1005	1/1	0.99	0.13	36,36,36,36	0
2	CL	B	1003	1/1	0.99	0.04	36,36,36,36	0

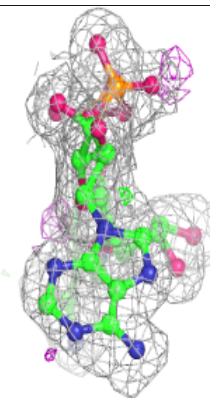
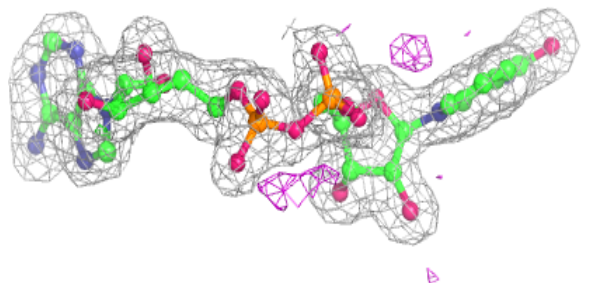
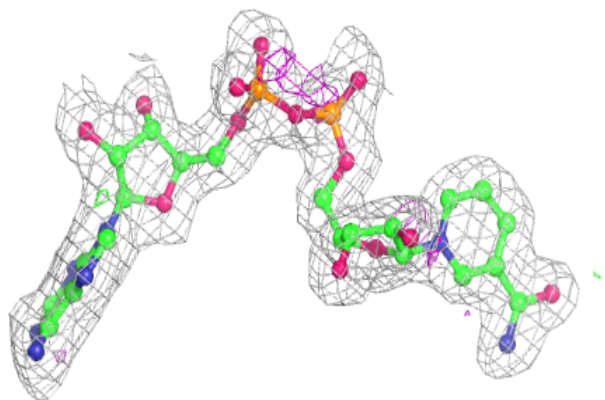
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

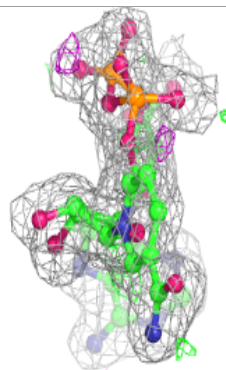
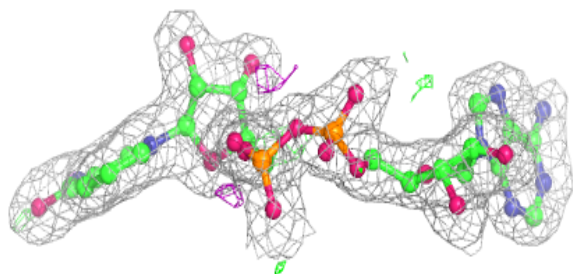
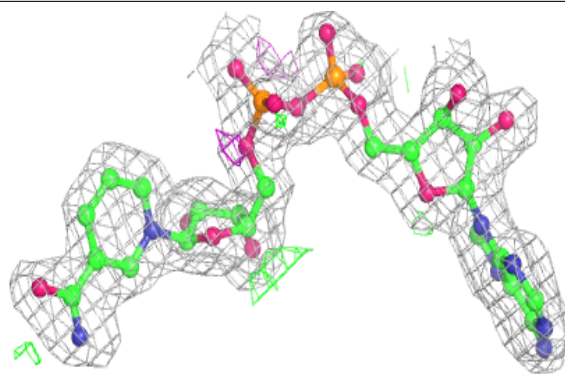
**Electron density around NAD C 3003:**

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

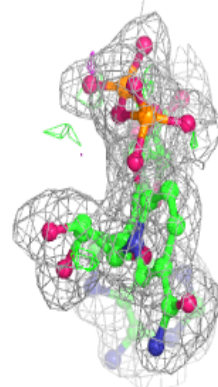
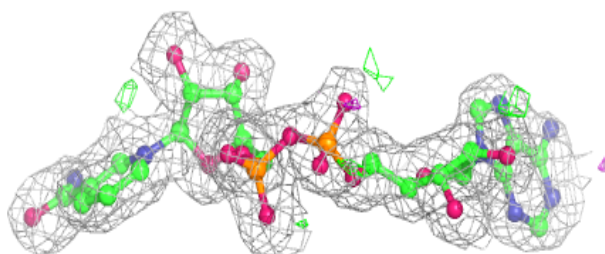
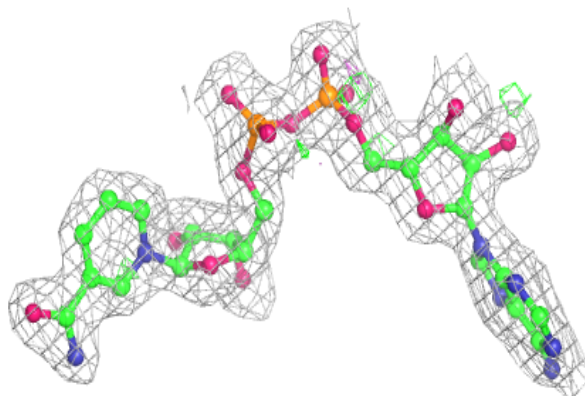


Electron density around NAD A 3001:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.