



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:44 AM UTC

PDB ID : 2W2L / pdb_00002w2l
Title : Crystal structure of the holo forms of Rhodotorula graminis D- mandelate dehydrogenase at 2.5Å.
Authors : Vachieri, S.G.; Cole, A.R.; Bagneris, C.; Baker, D.P.; Fewson, C.A.; Basak, A.K.
Deposited on : 2008-11-02
Resolution : 2.50 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

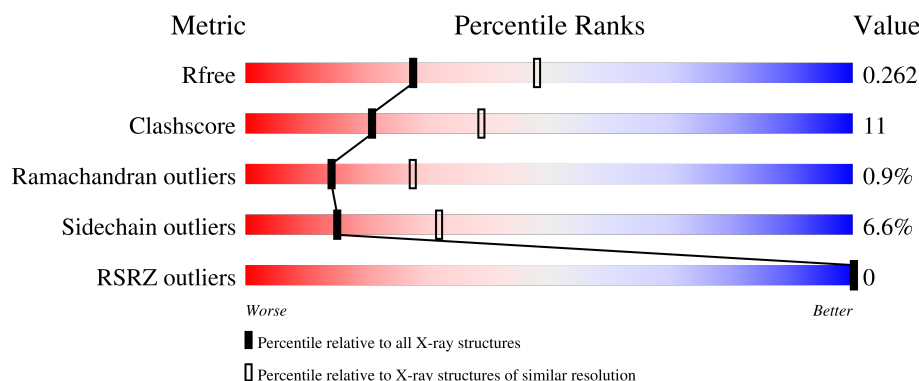
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

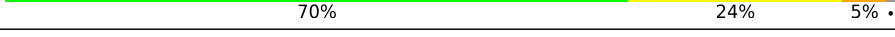
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	348	 72% 23% . .
1	B	348	 74% 24% ...
1	C	348	 73% 22% . .
2	D	348	 70% 24% 5% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11321 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 D-MANDELATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	22	0	0
			2664	1692	469	496	7			
1	B	345	Total	C	N	O	S	17	0	0
			2655	1686	468	495	6			
1	C	344	Total	C	N	O	S	34	0	0
			2650	1684	467	493	6			

- Molecule 2 is a protein called D-MANDELATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	345	Total	C	N	O	S	23	1	0
			2665	1693	471	494	7			

There is a discrepancy between the modelled and reference sequences:

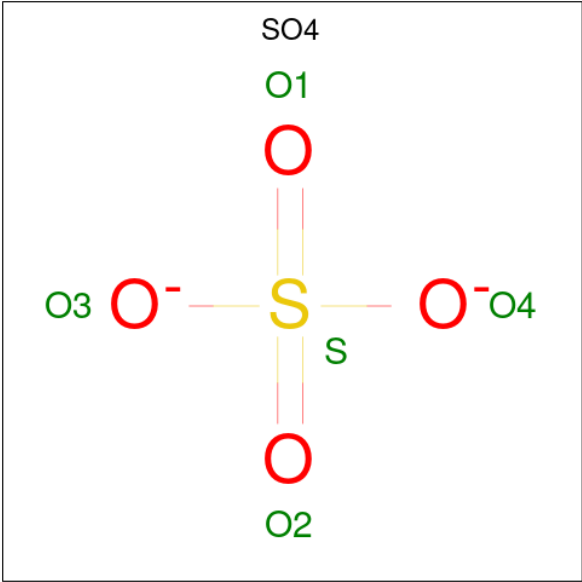
Chain	Residue	Modelled	Actual	Comment	Reference
D	73	ILE	LEU	conflict	UNP Q7LLW9

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



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

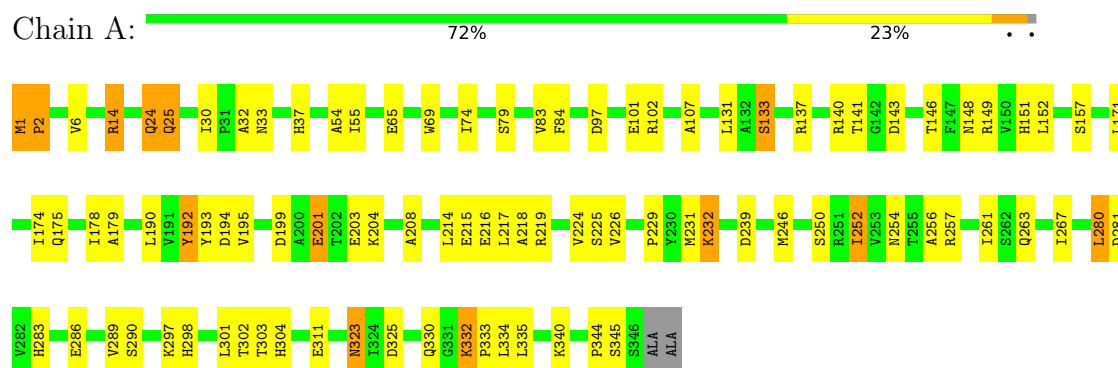
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	128	Total O 128 128	0	0
5	B	93	Total O 93 93	0	0
5	C	146	Total O 146 146	0	0
5	D	124	Total O 124 124	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: D-MANDELATE DEHYDROGENASE



● Molecule 2: D-MANDELATE DEHYDROGENASE

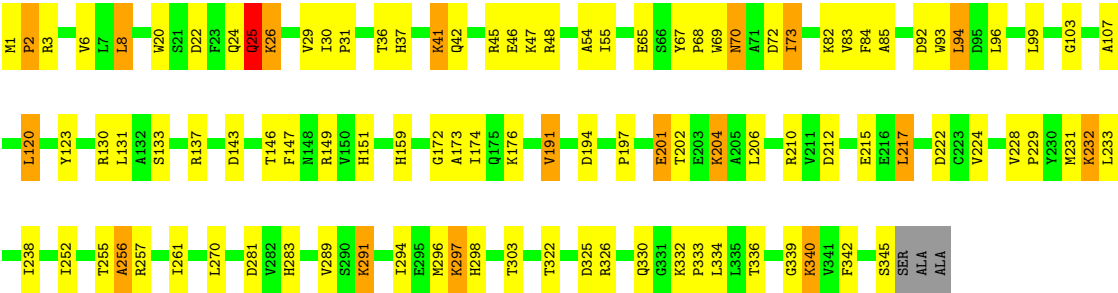
Chain D:

70%

24%

5%

 ●



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.10Å 110.15Å 79.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.50 48.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.28-2.50) 94.4 (48.28-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.265 0.182 , 0.262	Depositor DCC
R_{free} test set	2901 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 10.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.189 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11321	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8560e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.15	6/2721 (0.2%)	1.31	20/3687 (0.5%)
1	B	1.16	4/2712 (0.1%)	1.16	13/3674 (0.4%)
1	C	1.21	4/2707 (0.1%)	1.25	17/3668 (0.5%)
2	D	1.34	5/2725 (0.2%)	1.23	19/3691 (0.5%)
All	All	1.22	19/10865 (0.2%)	1.24	69/14720 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	D	0	1
All	All	0	6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	48	ARG	NE-CZ	34.96	1.71	1.33
1	C	45	ARG	CA-CB	-20.88	1.20	1.53
1	A	14	ARG	NE-CZ	18.52	1.53	1.33
1	B	232	LYS	CA-CB	-17.45	1.24	1.53
1	B	201	GLU	CA-CB	-16.92	1.26	1.53
2	D	291	LYS	CB-CG	16.39	2.01	1.52
1	C	48	ARG	CG-CD	-14.07	1.10	1.52
2	D	340	LYS	CB-CG	-10.02	1.22	1.52
1	A	232	LYS	CA-CB	-9.78	1.38	1.53
2	D	232	LYS	CB-CG	-9.72	1.23	1.52
2	D	201	GLU	CB-CG	9.70	1.81	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	LYS	CB-CG	-9.23	1.24	1.52
1	C	169	VAL	CA-CB	7.06	1.61	1.53
1	A	201	GLU	CB-CG	6.78	1.72	1.52
1	A	30	ILE	CA-C	-6.52	1.47	1.53
1	A	232	LYS	CB-CG	-6.25	1.33	1.52
1	C	201	GLU	CA-CB	5.78	1.62	1.53
1	B	48	ARG	CB-CG	-5.57	1.35	1.52
1	B	165	VAL	CA-CB	5.21	1.60	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH2	20.41	137.57	119.20
1	A	14	ARG	NE-CZ-NH1	-19.13	102.37	121.50
2	D	291	LYS	CA-CB-CG	-16.83	80.44	114.10
1	C	201	GLU	N-CA-CB	-15.57	86.15	110.28
1	A	232	LYS	CA-CB-CG	-11.97	90.17	114.10
1	A	14	ARG	CD-NE-CZ	11.05	139.87	124.40
1	A	232	LYS	CB-CA-C	10.58	127.35	110.95
2	D	26	LYS	N-CA-C	-10.50	88.44	110.80
1	C	48	ARG	CD-NE-CZ	9.79	138.10	124.40
2	D	204	LYS	CB-CG-CD	9.75	133.72	111.30
1	A	201	GLU	CB-CG-CD	-8.21	98.64	112.60
1	A	24	GLN	N-CA-C	8.13	123.75	112.45
1	A	1	MET	CA-C-N	-8.06	109.76	119.84
1	A	1	MET	C-N-CA	-8.06	109.76	119.84
1	C	6	VAL	N-CA-CB	8.04	124.50	111.23
1	C	45	ARG	N-CA-CB	7.89	123.13	109.72
1	A	201	GLU	CA-CB-CG	-7.53	99.05	114.10
1	C	35	THR	N-CA-C	-7.37	102.25	112.12
1	C	291	LYS	CA-CB-CG	-7.22	99.65	114.10
1	A	232	LYS	N-CA-CB	7.00	120.13	109.98
1	C	213	SER	N-CA-C	6.86	119.60	109.24
1	B	228	VAL	CA-C-N	-6.84	113.26	120.03
1	B	228	VAL	C-N-CA	-6.84	113.26	120.03
1	A	332	LYS	CA-C-N	-6.63	113.96	120.52
1	A	332	LYS	C-N-CA	-6.63	113.96	120.52
2	D	25	GLN	CA-C-N	6.56	134.06	121.54
2	D	25	GLN	C-N-CA	6.56	134.06	121.54
1	B	155	GLY	N-CA-C	6.52	120.53	112.64
1	B	30	ILE	CB-CA-C	-6.28	103.96	111.18
1	A	148	ASN	N-CA-C	6.14	117.97	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	SER	N-CA-C	6.08	121.63	113.72
2	D	30	ILE	CA-C-N	-6.08	113.68	119.76
2	D	30	ILE	C-N-CA	-6.08	113.68	119.76
2	D	336	THR	CA-C-N	6.04	126.01	120.03
2	D	336	THR	C-N-CA	6.04	126.01	120.03
1	C	69	TRP	CA-C-N	6.03	133.05	121.54
1	C	69	TRP	C-N-CA	6.03	133.05	121.54
1	B	154	ILE	CA-C-N	6.02	126.79	119.99
1	B	154	ILE	C-N-CA	6.02	126.79	119.99
2	D	25	GLN	N-CA-C	-5.98	103.94	111.11
1	B	213	SER	N-CA-C	5.95	118.23	109.24
1	C	70	ASN	CB-CA-C	-5.82	98.84	110.42
2	D	332	LYS	CA-C-N	-5.79	114.64	120.31
2	D	332	LYS	C-N-CA	-5.79	114.64	120.31
1	B	261	ILE	N-CA-C	-5.76	100.18	108.53
1	B	3	ARG	CA-C-N	5.73	125.71	120.21
1	B	3	ARG	C-N-CA	5.73	125.71	120.21
1	A	143	ASP	CA-C-N	5.58	126.82	119.84
1	A	143	ASP	C-N-CA	5.58	126.82	119.84
2	D	173	ALA	N-CA-C	5.56	117.78	111.11
1	C	80	SER	N-CA-C	5.44	122.38	110.80
2	D	297	LYS	N-CA-C	5.43	116.89	111.07
1	B	232	LYS	N-CA-CB	5.39	119.60	110.49
1	A	30	ILE	CA-C-N	5.34	125.50	119.90
1	A	30	ILE	C-N-CA	5.34	125.50	119.90
1	C	5	ARG	CA-C-N	5.21	131.35	121.97
1	C	5	ARG	C-N-CA	5.21	131.35	121.97
1	B	77	LEU	CA-C-N	-5.20	114.88	120.03
1	B	77	LEU	C-N-CA	-5.20	114.88	120.03
2	D	222	ASP	N-CA-C	-5.20	107.07	113.41
2	D	143	ASP	CA-C-N	5.20	126.34	119.84
2	D	143	ASP	C-N-CA	5.20	126.34	119.84
1	A	25	GLN	N-CA-C	5.18	121.84	110.80
1	A	192	TYR	N-CA-C	5.17	117.04	109.24
2	D	94	LEU	N-CA-C	5.17	116.83	108.41
1	C	117	THR	N-CA-C	-5.08	105.83	112.23
2	D	212	ASP	N-CA-C	5.08	117.94	111.69
1	C	336	THR	CB-CA-C	-5.07	104.57	111.21
1	C	45	ARG	CB-CA-C	5.05	119.23	110.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	24	GLN	Peptide
1	C	48	ARG	Sidechain
1	C	5	ARG	Peptide
1	C	79	SER	Peptide
2	D	25	GLN	Peptide

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	2664	0	2664	69	0
1	B	2655	0	2649	48	0
1	C	2650	0	2648	52	0
2	D	2665	0	2668	82	0
3	A	44	0	26	4	0
3	B	44	0	26	4	0
3	C	44	0	26	2	0
3	D	44	0	26	9	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	128	0	0	6	0
5	B	93	0	0	1	0
5	C	146	0	0	4	0
5	D	124	0	0	12	0
All	All	11321	0	10733	237	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 11.

All (237) 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)
3:D:1346:NAD:H2D	5:D:2035:HOH:O	1.42	1.14
1:C:270:LEU:HB3	1:C:296:MET:HE1	1.29	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:LEU:HB3	2:D:296:MET:HE1	1.31	1.08
2:D:1:MET:HB3	2:D:2:PRO:HA	1.33	1.05
1:A:37:HIS:HE1	5:A:2042:HOH:O	1.36	1.05
2:D:107:ALA:HB2	2:D:334:LEU:HD13	1.42	1.01
1:A:193:TYR:CE2	1:A:214:LEU:HD23	2.02	0.94
1:A:229:PRO:HD3	3:A:1347:NAD:H52A	1.50	0.93
1:C:20:TRP:CE3	1:C:321:MET:HE2	2.05	0.92
2:D:70:ASN:HD21	2:D:73:ILE:HG22	1.31	0.91
1:A:193:TYR:HE2	1:A:214:LEU:CD2	1.86	0.88
1:A:193:TYR:HE2	1:A:214:LEU:HD23	1.37	0.87
2:D:270:LEU:CB	2:D:296:MET:HE1	2.06	0.86
2:D:70:ASN:ND2	2:D:73:ILE:HG22	1.92	0.85
2:D:8:LEU:CD2	2:D:31:PRO:HA	2.10	0.82
2:D:283:HIS:HD2	5:D:2108:HOH:O	1.63	0.81
1:A:193:TYR:OH	1:B:25:GLN:HG3	1.80	0.81
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.63	0.81
1:C:36:THR:HG23	1:C:39:GLY:H	1.47	0.80
2:D:8:LEU:HD23	2:D:31:PRO:HA	1.63	0.79
2:D:233:LEU:CB	5:D:2085:HOH:O	2.31	0.79
2:D:281:ASP:C	5:D:2100:HOH:O	2.25	0.79
2:D:2:PRO:HD2	2:D:3:ARG:H	1.46	0.79
1:C:286:GLU:OE1	1:C:304:HIS:HD2	1.67	0.78
2:D:70:ASN:ND2	2:D:73:ILE:CG2	2.46	0.77
1:C:20:TRP:HE3	1:C:321:MET:HE2	1.49	0.77
1:A:286:GLU:OE1	1:A:304:HIS:HD2	1.69	0.76
1:C:228:VAL:O	3:C:1346:NAD:O3D	2.06	0.74
2:D:194:ASP:OD2	3:D:1346:NAD:H1B	1.88	0.74
1:A:323:ASN:HD21	1:A:335:LEU:H	1.34	0.73
1:A:323:ASN:ND2	1:A:335:LEU:H	1.85	0.73
1:C:270:LEU:CB	1:C:296:MET:HE1	2.13	0.73
2:D:174:ILE:HG13	3:D:1346:NAD:O1N	1.90	0.72
1:B:259:PRO:HA	1:B:284:GLU:HG3	1.72	0.71
2:D:255:THR:O	3:D:1346:NAD:H2N	1.90	0.71
1:B:192:TYR:OH	1:B:203:GLU:OE2	2.07	0.71
2:D:283:HIS:CE1	5:D:2100:HOH:O	2.44	0.70
1:A:203:GLU:HG2	1:A:208:ALA:HB3	1.73	0.70
1:A:226:VAL:HG21	1:A:261:ILE:HD11	1.73	0.69
1:B:286:GLU:OE1	1:B:304:HIS:HD2	1.76	0.68
1:A:37:HIS:CE1	5:A:2042:HOH:O	2.23	0.68
1:A:65:GLU:OE1	1:A:65:GLU:N	2.26	0.67
1:A:239:ASP:HB3	5:A:2092:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:ARG:NH1	5:D:2024:HOH:O	2.26	0.66
1:C:224:VAL:HB	1:C:252:ILE:HG13	1.77	0.65
1:A:1:MET:HB3	1:A:2:PRO:CD	2.26	0.65
1:A:224:VAL:HB	1:A:252:ILE:HG13	1.78	0.64
2:D:70:ASN:C	2:D:70:ASN:HD22	2.05	0.64
2:D:281:ASP:O	5:D:2100:HOH:O	2.15	0.64
1:A:194:ASP:OD2	3:A:1347:NAD:H1B	1.99	0.63
1:C:64:THR:HB	5:C:2033:HOH:O	1.99	0.62
2:D:120:LEU:O	2:D:123:TYR:HB3	1.98	0.62
1:A:193:TYR:OH	1:B:25:GLN:CG	2.46	0.62
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.65	0.62
1:A:193:TYR:CE2	1:A:214:LEU:CD2	2.72	0.62
2:D:96:LEU:HD21	2:D:339:GLY:HA3	1.82	0.62
1:B:55:ILE:HD13	1:B:69:TRP:HH2	1.65	0.61
2:D:270:LEU:HB3	2:D:296:MET:CE	2.19	0.61
1:C:5:ARG:NH2	1:C:49:TYR:O	2.34	0.60
2:D:1:MET:HB3	2:D:2:PRO:CA	2.21	0.60
2:D:2:PRO:HD2	2:D:3:ARG:N	2.14	0.60
1:C:70:ASN:HB3	1:C:73:LEU:H	1.65	0.59
2:D:107:ALA:HB2	2:D:334:LEU:CD1	2.27	0.59
2:D:131:LEU:HD22	2:D:298:HIS:CD2	2.37	0.59
2:D:22:ASP:O	2:D:25:GLN:HB3	2.02	0.59
1:A:107:ALA:HB2	1:A:334:LEU:HD13	1.84	0.59
1:B:131:LEU:HD22	1:B:298:HIS:CD2	2.38	0.59
1:A:55:ILE:HD13	1:A:69:TRP:CH2	2.38	0.58
2:D:93:TRP:CD1	2:D:93:TRP:H	2.19	0.58
1:B:159:HIS:HD2	1:C:311:GLU:OE2	1.87	0.57
1:A:192:TYR:OH	1:A:203:GLU:OE2	2.22	0.56
2:D:20:TRP:O	2:D:24:GLN:HG3	2.05	0.56
2:D:41:LYS:NZ	2:D:72:ASP:OD2	2.35	0.56
1:B:55:ILE:HD13	1:B:69:TRP:CH2	2.41	0.56
1:B:167:GLY:HA3	1:B:221:SER:OG	2.05	0.56
2:D:8:LEU:HD21	2:D:31:PRO:HA	1.86	0.55
1:A:311:GLU:OE2	2:D:159:HIS:HD2	1.89	0.55
1:C:107:ALA:HB2	1:C:334:LEU:HD13	1.88	0.55
1:C:229:PRO:HG2	1:C:231:MET:HE3	1.88	0.55
1:A:229:PRO:HD3	3:A:1347:NAD:C5B	2.29	0.55
2:D:84:PHE:HD2	2:D:85:ALA:N	2.05	0.55
1:B:140:ARG:HH11	1:B:140:ARG:CG	2.19	0.55
2:D:1:MET:CB	2:D:2:PRO:HA	2.13	0.55
1:B:195:VAL:HG23	1:B:196:ALA:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD13	1:B:66:SER:HB3	1.89	0.54
2:D:228:VAL:O	3:D:1346:NAD:O3D	2.18	0.54
1:A:193:TYR:CD2	1:A:214:LEU:HD23	2.42	0.54
1:B:137:ARG:HD3	1:C:140:ARG:NE	2.23	0.54
1:C:84:PHE:HD2	1:C:85:ALA:N	2.06	0.53
2:D:82:LYS:HE3	2:D:345:SER:OG	2.08	0.53
1:B:175:GLN:HE22	1:B:225:SER:CB	2.22	0.53
1:A:55:ILE:HD13	1:A:69:TRP:HH2	1.72	0.52
2:D:103:GLY:HA2	2:D:342:PHE:CE2	2.45	0.52
2:D:283:HIS:HB3	5:D:2104:HOH:O	2.08	0.52
1:A:286:GLU:OE1	1:A:304:HIS:CD2	2.57	0.52
2:D:70:ASN:ND2	2:D:73:ILE:HG23	2.24	0.51
2:D:333:PRO:HB3	5:D:2121:HOH:O	2.10	0.51
1:C:286:GLU:OE1	1:C:304:HIS:CD2	2.56	0.51
1:B:194:ASP:OD2	3:B:1347:NAD:H1B	2.10	0.51
1:C:20:TRP:HE3	1:C:321:MET:CE	2.22	0.51
1:B:257:ARG:NH1	4:B:1348:SO4:O1	2.42	0.50
1:A:218:ALA:HB1	1:A:246:MET:HG3	1.93	0.50
1:A:239:ASP:CB	5:A:2092:HOH:O	2.57	0.50
1:C:203:GLU:HG2	1:C:208:ALA:HB3	1.94	0.50
2:D:229:PRO:HD3	3:D:1346:NAD:H52A	1.94	0.50
1:B:94:LEU:HD11	1:B:99:LEU:HD22	1.93	0.49
2:D:325:ASP:OD1	2:D:330:GLN:NE2	2.46	0.49
1:A:325:ASP:OD1	1:A:330:GLN:NE2	2.44	0.49
2:D:25:GLN:HA	2:D:25:GLN:OE1	2.13	0.49
2:D:2:PRO:CD	2:D:3:ARG:N	2.76	0.49
2:D:191:VAL:HG23	2:D:217:LEU:HD12	1.95	0.49
1:C:326:ARG:HA	1:C:330:GLN:HB2	1.95	0.49
2:D:224:VAL:HB	2:D:252:ILE:HG13	1.95	0.49
2:D:283:HIS:CD2	5:D:2108:HOH:O	2.50	0.49
1:B:49:TYR:HB2	5:B:2010:HOH:O	2.13	0.48
1:C:133:SER:O	1:C:137:ARG:HG2	2.12	0.48
1:B:293:LEU:HB3	1:B:299:VAL:HG11	1.95	0.48
1:B:22:ASP:O	1:B:26:LYS:HG3	2.14	0.48
1:C:5:ARG:HD2	1:C:28:GLU:OE1	2.13	0.48
2:D:2:PRO:CD	2:D:3:ARG:H	2.19	0.48
2:D:54:ALA:HA	2:D:83:VAL:O	2.14	0.48
2:D:137:ARG:NH2	2:D:297:LYS:O	2.45	0.48
2:D:172:GLY:HA3	3:D:1346:NAD:H4B	1.95	0.48
2:D:322:THR:O	2:D:326:ARG:HG3	2.14	0.48
1:A:281:ASP:OD1	1:A:302:THR:OG1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:HG22	1:B:67:TYR:CZ	2.49	0.47
1:A:133:SER:O	1:A:137:ARG:HG3	2.13	0.47
1:A:6:VAL:HG22	1:A:54:ALA:HB3	1.96	0.47
2:D:238:ILE:HB	2:D:261:ILE:HG12	1.95	0.47
1:C:165:VAL:CG1	1:C:191:VAL:HG13	2.44	0.47
1:A:97:ASP:O	1:A:101:GLU:HG2	2.15	0.47
1:A:101:GLU:HG3	5:A:2052:HOH:O	2.15	0.47
2:D:55:ILE:HD13	2:D:69:TRP:CH2	2.49	0.47
1:A:174:ILE:O	1:A:178:ILE:HG13	2.15	0.47
1:A:151:HIS:HD2	2:D:303:THR:O	1.97	0.47
1:B:227:SER:HA	1:B:256:ALA:HB2	1.96	0.46
2:D:84:PHE:C	2:D:84:PHE:CD2	2.92	0.46
1:C:36:THR:CG2	1:C:39:GLY:H	2.21	0.46
1:B:87:ALA:HB1	1:B:316:PHE:CD2	2.49	0.46
2:D:22:ASP:O	2:D:26:LYS:HB2	2.16	0.46
2:D:283:HIS:CD2	2:D:289:VAL:HG22	2.51	0.46
1:A:140:ARG:NH2	2:D:294:ILE:O	2.48	0.46
1:C:138:ALA:HB2	1:C:150:VAL:HG11	1.96	0.46
2:D:96:LEU:HD21	2:D:339:GLY:CA	2.44	0.46
2:D:174:ILE:CG1	3:D:1346:NAD:O1N	2.61	0.46
1:A:84:PHE:CD2	1:A:84:PHE:C	2.89	0.46
1:B:231:MET:O	1:B:232:LYS:C	2.59	0.46
2:D:172:GLY:O	2:D:176:LYS:HG3	2.15	0.46
1:B:191:VAL:HA	1:B:209:GLU:O	2.16	0.46
1:C:74:ILE:HD13	1:C:99:LEU:HB2	1.98	0.45
1:C:258:GLY:HA3	1:C:283:HIS:C	2.41	0.45
1:B:304:HIS:HE1	3:B:1347:NAD:C7N	2.30	0.45
1:A:289:VAL:HG11	1:A:301:LEU:HD13	1.98	0.45
1:C:20:TRP:CE3	1:C:321:MET:CE	2.89	0.45
1:A:171:LEU:O	1:A:171:LEU:HG	2.17	0.45
1:A:195:VAL:HB	1:B:21:SER:HB3	1.98	0.45
1:A:280:LEU:HB2	1:A:301:LEU:HD23	1.99	0.45
1:B:41:LYS:HB3	1:B:73:LEU:HD13	1.99	0.45
1:B:340:LYS:HB3	1:B:342:PHE:CE1	2.51	0.45
1:C:198:ALA:HB3	1:C:203:GLU:HG3	1.97	0.45
1:A:256:ALA:HA	3:A:1347:NAD:H1D	1.98	0.45
1:A:137:ARG:NH2	1:A:297:LYS:O	2.50	0.45
2:D:70:ASN:ND2	2:D:70:ASN:C	2.74	0.45
1:C:74:ILE:HG22	1:C:102:ARG:HD2	1.99	0.44
1:C:279:GLY:HA2	1:C:300:THR:O	2.17	0.44
1:A:131:LEU:HD22	1:A:298:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:HA	2:D:147:PHE:CE1	2.52	0.44
1:B:9:LEU:HD22	1:B:34:LEU:HD11	1.99	0.44
1:B:81:LEU:HD23	1:B:104:VAL:HG21	1.99	0.44
1:C:137:ARG:HG2	1:C:137:ARG:H	1.59	0.44
1:C:84:PHE:C	1:C:84:PHE:CD2	2.95	0.44
2:D:37:HIS:HE1	2:D:73:ILE:HG21	1.82	0.44
1:A:175:GLN:NE2	1:A:225:SER:OG	2.37	0.44
1:C:81:LEU:HD12	1:C:82:LYS:H	1.83	0.44
1:B:304:HIS:CE1	3:B:1347:NAD:C7N	3.01	0.44
2:D:42:GLN:OE1	2:D:42:GLN:HA	2.15	0.43
2:D:197:PRO:HB3	2:D:210:ARG:NH1	2.33	0.43
1:B:133:SER:OG	1:C:136:GLU:OE1	2.33	0.43
1:B:323:ASN:ND2	1:B:335:LEU:H	2.16	0.43
2:D:8:LEU:HD22	2:D:29:VAL:CG1	2.48	0.43
1:B:147:PHE:C	1:B:147:PHE:CD2	2.96	0.43
1:C:130:ARG:NH1	5:C:2056:HOH:O	2.36	0.43
2:D:84:PHE:HD2	2:D:84:PHE:C	2.26	0.43
1:A:54:ALA:HA	1:A:83:VAL:O	2.19	0.43
1:C:209:GLU:CD	1:C:220:ARG:HH22	2.26	0.43
2:D:25:GLN:NE2	5:D:2015:HOH:O	2.52	0.43
2:D:256:ALA:HA	3:D:1346:NAD:H1D	2.01	0.43
1:B:238:ILE:HG23	1:B:242:PHE:CD2	2.53	0.43
1:C:255:THR:O	3:C:1346:NAD:H2N	2.19	0.43
1:B:256:ALA:HA	3:B:1347:NAD:H1D	2.01	0.42
2:D:146:THR:HG23	2:D:149:ARG:NH2	2.34	0.42
1:A:303:THR:O	2:D:151:HIS:HD2	2.02	0.42
1:C:110:ARG:CZ	1:C:110:ARG:HB3	2.49	0.42
1:C:147:PHE:C	1:C:147:PHE:CD2	2.97	0.42
1:B:151:HIS:CD2	1:C:304:HIS:O	2.72	0.42
1:C:238:ILE:HB	1:C:261:ILE:HA	2.01	0.42
2:D:322:THR:HG22	2:D:326:ARG:HD3	2.00	0.42
1:A:179:ALA:HB1	1:A:190:LEU:HD22	2.01	0.42
1:A:333:PRO:HB3	5:A:2124:HOH:O	2.19	0.42
1:B:102:ARG:HE	1:B:102:ARG:HB3	1.68	0.42
1:B:3:ARG:HA	1:B:4:PRO:HD2	1.95	0.42
1:C:257:ARG:HG3	5:C:2112:HOH:O	2.19	0.42
2:D:322:THR:HG22	2:D:326:ARG:CD	2.49	0.42
2:D:133:SER:O	2:D:137:ARG:HG3	2.20	0.42
1:A:65:GLU:H	1:A:65:GLU:CD	2.22	0.42
1:A:283:HIS:CD2	1:A:289:VAL:HG13	2.55	0.42
1:C:72:ASP:O	1:C:76:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:THR:O	2:D:206:LEU:HG	2.20	0.42
1:B:56:ILE:O	1:B:56:ILE:HG23	2.20	0.42
1:C:38:ASP:O	1:C:42:GLN:HG2	2.19	0.42
1:A:254:ASN:HB2	1:A:261:ILE:HD12	2.02	0.41
1:A:330:GLN:O	1:A:332:LYS:HG3	2.19	0.41
2:D:94:LEU:HD11	2:D:99:LEU:HD22	2.03	0.41
1:B:74:ILE:CG2	1:B:102:ARG:HG3	2.50	0.41
1:B:136:GLU:OE2	1:C:123:TYR:OH	2.30	0.41
1:C:47:LYS:HE3	5:C:2014:HOH:O	2.20	0.41
2:D:6:VAL:HG22	2:D:54:ALA:HB3	2.03	0.41
1:A:84:PHE:C	1:A:84:PHE:HD2	2.28	0.41
1:A:263:GLN:NE2	1:A:290:SER:HB2	2.36	0.41
1:A:283:HIS:HE1	1:A:302:THR:O	2.03	0.41
1:B:138:ALA:HB2	1:B:150:VAL:HG21	2.03	0.41
1:A:246:MET:HE2	1:A:250:SER:OG	2.21	0.41
1:B:151:HIS:HD2	1:C:303:THR:O	2.04	0.41
1:A:263:GLN:O	1:A:267:ILE:HG13	2.20	0.41
1:A:1:MET:CB	1:A:2:PRO:CD	2.98	0.41
1:A:141:THR:HG21	1:A:146:THR:HG21	2.02	0.41
2:D:67:TYR:HB3	2:D:68:PRO:HA	2.03	0.41
1:B:6:VAL:HG22	1:B:54:ALA:HB3	2.01	0.41
1:C:87:ALA:HB1	1:C:316:PHE:CG	2.56	0.40
1:A:193:TYR:HE2	1:A:214:LEU:HD21	1.81	0.40
1:A:323:ASN:HD22	1:A:323:ASN:HA	1.77	0.40
2:D:130:ARG:NH1	5:D:2054:HOH:O	2.50	0.40
1:C:40:PHE:CD2	1:C:73:LEU:HD11	2.56	0.40
1:A:79:SER:HB2	1:C:216:GLU:OE1	2.21	0.40
1:C:69:TRP:HA	1:C:73:LEU:HD23	2.03	0.40
1:A:32:ALA:O	1:A:33:ASN:C	2.64	0.40
1:A:218:ALA:O	1:A:246:MET:HA	2.21	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	344/348 (99%)	318 (92%)	22 (6%)	4 (1%)	10	20
1	B	343/348 (99%)	321 (94%)	18 (5%)	4 (1%)	10	20
1	C	342/348 (98%)	322 (94%)	17 (5%)	3 (1%)	14	27
2	D	344/348 (99%)	326 (95%)	16 (5%)	2 (1%)	21	38
All	All	1373/1392 (99%)	1287 (94%)	73 (5%)	13 (1%)	14	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	C	6	VAL
1	C	80	SER
1	B	3	ARG
1	B	303	THR
2	D	2	PRO
1	A	216	GLU
1	B	232	LYS
1	C	70	ASN
2	D	256	ALA
1	A	2	PRO
1	A	344	PRO
1	B	306	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	278/279 (100%)	259 (93%)	19 (7%)	14	31
1	B	277/279 (99%)	261 (94%)	16 (6%)	18	38
1	C	276/279 (99%)	258 (94%)	18 (6%)	15	32
2	D	278/279 (100%)	258 (93%)	20 (7%)	13	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1109/1116 (99%)	1036 (93%)	73 (7%)	15	32

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	102	ARG
1	A	133	SER
1	A	149	ARG
1	A	152	LEU
1	A	157	SER
1	A	199	ASP
1	A	201	GLU
1	A	204	LYS
1	A	215	GLU
1	A	217	LEU
1	A	219	ARG
1	A	231	MET
1	A	232	LYS
1	A	252	ILE
1	A	257	ARG
1	A	280	LEU
1	A	323	ASN
1	A	345	SER
1	B	11	ASP
1	B	35	THR
1	B	57	LYS
1	B	72	ASP
1	B	79	SER
1	B	133	SER
1	B	137	ARG
1	B	140	ARG
1	B	145	GLU
1	B	156	LYS
1	B	204	LYS
1	B	217	LEU
1	B	219	ARG
1	B	232	LYS
1	B	272	SER
1	B	340	LYS
1	C	2	PRO
1	C	5	ARG

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Mol	Chain	Res	Type
1	C	16	LEU
1	C	25	GLN
1	C	46	GLU
1	C	47	LYS
1	C	64	THR
1	C	65	GLU
1	C	84	PHE
1	C	92	ASP
1	C	120	LEU
1	C	125	ILE
1	C	137	ARG
1	C	191	VAL
1	C	257	ARG
1	C	291	LYS
1	C	295	GLU
1	C	345	SER
2	D	8	LEU
2	D	36	THR
2	D	41	LYS
2	D	46	GLU
2	D	47	LYS
2	D	65	GLU
2	D	70	ASN
2	D	73	ILE
2	D	92	ASP
2	D	120	LEU
2	D	191	VAL
2	D	201	GLU
2	D	204	LYS
2	D	215	GLU
2	D	217	LEU
2	D	231	MET
2	D	232	LYS
2	D	257	ARG
2	D	291	LYS
2	D	340	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	37	HIS

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Mol	Chain	Res	Type
1	A	151	HIS
1	A	164	HIS
1	A	283	HIS
1	A	298	HIS
1	A	304	HIS
1	A	323	ASN
1	B	15	HIS
1	B	24	GLN
1	B	25	GLN
1	B	33	ASN
1	B	37	HIS
1	B	151	HIS
1	B	159	HIS
1	B	175	GLN
1	B	235	HIS
1	B	304	HIS
1	B	323	ASN
1	C	25	GLN
1	C	37	HIS
1	C	76	HIS
1	C	100	ASN
1	C	151	HIS
1	C	159	HIS
1	C	235	HIS
1	C	298	HIS
1	C	304	HIS
2	D	33	ASN
2	D	37	HIS
2	D	62	ASN
2	D	70	ASN
2	D	151	HIS
2	D	159	HIS
2	D	160	ASN
2	D	175	GLN
2	D	283	HIS
2	D	298	HIS
2	D	304	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAD	C	1346	-	46,48,48	1.93	9 (19%)	64,73,73	1.96	17 (26%)
4	SO4	D	1347	-	4,4,4	0.29	0	6,6,6	0.40	0
3	NAD	D	1346	-	46,48,48	1.99	8 (17%)	64,73,73	1.81	14 (21%)
3	NAD	B	1347	-	46,48,48	1.68	6 (13%)	64,73,73	1.81	15 (23%)
3	NAD	A	1347	-	46,48,48	1.87	7 (15%)	64,73,73	1.85	11 (17%)
4	SO4	A	1348	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	B	1348	-	4,4,4	0.30	0	6,6,6	0.75	0
4	SO4	C	1347	-	4,4,4	0.33	0	6,6,6	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	1346	-	-	13/30/62/62	0/5/5/5
3	NAD	C	1346	-	-	13/30/62/62	0/5/5/5
3	NAD	B	1347	-	-	11/30/62/62	0/5/5/5
3	NAD	A	1347	-	-	9/30/62/62	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1346	NAD	O7N-C7N	9.78	1.42	1.24
3	A	1347	NAD	O7N-C7N	9.33	1.41	1.24
3	C	1346	NAD	O7N-C7N	9.03	1.40	1.24
3	B	1347	NAD	O7N-C7N	8.64	1.40	1.24
3	D	1346	NAD	PN-O3	4.17	1.64	1.59
3	C	1346	NAD	C2N-N1N	3.76	1.39	1.35
3	C	1346	NAD	PN-O3	3.72	1.63	1.59
3	A	1347	NAD	C2N-N1N	3.64	1.39	1.35
3	D	1346	NAD	C2A-N1A	3.04	1.39	1.33
3	D	1346	NAD	C2A-N3A	2.99	1.39	1.33
3	C	1346	NAD	C2A-N1A	2.94	1.39	1.33
3	D	1346	NAD	C2N-N1N	2.94	1.38	1.35
3	A	1347	NAD	O4D-C1D	2.86	1.44	1.40
3	A	1347	NAD	C2A-N3A	2.83	1.39	1.33
3	B	1347	NAD	C2A-N1A	2.83	1.39	1.33
3	C	1346	NAD	PA-O3	2.49	1.62	1.59
3	D	1346	NAD	PA-O3	2.48	1.62	1.59
3	B	1347	NAD	C2A-N3A	2.41	1.38	1.33
3	C	1346	NAD	C2A-N3A	2.36	1.38	1.33
3	B	1347	NAD	O4D-C1D	2.32	1.43	1.40
3	A	1347	NAD	C8A-N7A	2.28	1.36	1.31
3	A	1347	NAD	C2A-N1A	2.25	1.37	1.33
3	C	1346	NAD	C8A-N7A	2.24	1.36	1.31
3	B	1347	NAD	C5A-N7A	-2.21	1.35	1.39
3	C	1346	NAD	C5A-N7A	-2.21	1.35	1.39
3	A	1347	NAD	C5A-N7A	-2.15	1.35	1.39
3	D	1346	NAD	O4D-C1D	2.13	1.43	1.40
3	C	1346	NAD	O4D-C1D	2.09	1.43	1.40
3	B	1347	NAD	C8A-N7A	2.06	1.35	1.31
3	D	1346	NAD	C8A-N7A	2.06	1.35	1.31

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1347	NAD	N3A-C2A-N1A	-6.80	118.29	128.58
3	B	1347	NAD	N3A-C2A-N1A	-5.87	119.69	128.58
3	C	1346	NAD	N3A-C2A-N1A	-5.63	120.06	128.58
3	D	1346	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
3	C	1346	NAD	C5A-C4A-N3A	-5.50	119.14	126.72
3	D	1346	NAD	C5A-C4A-N3A	-4.69	120.27	126.72
3	A	1347	NAD	C5A-C4A-N3A	-4.63	120.34	126.72
3	B	1347	NAD	C3N-C7N-N7N	4.56	123.35	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1347	NAD	C3N-C7N-N7N	4.18	122.89	117.74
3	C	1346	NAD	C3N-C7N-N7N	4.16	122.87	117.74
3	A	1347	NAD	C2A-N3A-C4A	3.90	121.36	111.83
3	C	1346	NAD	C2A-N3A-C4A	3.83	121.19	111.83
3	A	1347	NAD	N9A-C8A-N7A	-3.76	108.61	113.94
3	B	1347	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
3	D	1346	NAD	N9A-C8A-N7A	-3.60	108.83	113.94
3	D	1346	NAD	N3A-C4A-N9A	3.58	133.26	127.17
3	B	1347	NAD	C5A-C4A-N3A	-3.55	121.83	126.72
3	C	1346	NAD	C5A-N7A-C8A	3.53	109.00	103.45
3	D	1346	NAD	O3-PN-O1N	-3.41	100.44	110.70
3	C	1346	NAD	O3-PN-O1N	-3.39	100.52	110.70
3	B	1347	NAD	O7N-C7N-C3N	-3.34	115.52	119.60
3	C	1346	NAD	O3D-C3D-C2D	-3.34	101.12	111.82
3	D	1346	NAD	C6N-N1N-C2N	-3.33	119.05	121.88
3	A	1347	NAD	O7N-C7N-C3N	-3.29	115.57	119.60
3	B	1347	NAD	C5A-N7A-C8A	3.26	108.58	103.45
3	A	1347	NAD	N3A-C4A-N9A	3.24	132.69	127.17
3	D	1346	NAD	C2A-N3A-C4A	3.24	119.74	111.83
3	D	1346	NAD	C5A-N7A-C8A	3.13	108.37	103.45
3	A	1347	NAD	C4D-O4D-C1D	-3.10	107.08	109.92
3	C	1346	NAD	N3A-C4A-N9A	3.10	132.44	127.17
3	C	1346	NAD	N9A-C8A-N7A	-3.09	109.55	113.94
3	A	1347	NAD	C5A-N7A-C8A	3.08	108.29	103.45
3	B	1347	NAD	O2A-PA-O3	3.01	115.41	107.27
3	B	1347	NAD	C2A-N3A-C4A	2.91	118.95	111.83
3	C	1346	NAD	C4A-C5A-N7A	-2.90	107.26	110.58
3	C	1346	NAD	C2D-C3D-C4D	2.88	108.18	102.61
3	C	1346	NAD	O7N-C7N-C3N	-2.85	116.11	119.60
3	C	1346	NAD	C3B-C2B-C1B	2.77	106.71	101.46
3	D	1346	NAD	C3N-C7N-N7N	2.63	120.98	117.74
3	B	1347	NAD	O3-PA-O1A	-2.59	102.92	110.70
3	D	1346	NAD	C4D-O4D-C1D	-2.57	107.57	109.92
3	C	1346	NAD	C6A-C5A-C4A	2.47	120.55	117.18
3	D	1346	NAD	C6A-C5A-C4A	2.44	120.51	117.18
3	B	1347	NAD	C4A-C5A-N7A	-2.39	107.85	110.58
3	C	1346	NAD	C5A-C4A-N9A	2.39	108.41	105.81
3	D	1346	NAD	O2A-PA-O3	2.33	113.56	107.27
3	C	1346	NAD	C6N-N1N-C2N	-2.31	119.91	121.88
3	D	1346	NAD	O2A-PA-O5B	2.31	118.03	107.57
3	C	1346	NAD	O2A-PA-O5B	2.28	117.92	107.57
3	B	1347	NAD	C5A-C6A-N6A	-2.24	117.75	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1347	NAD	O2N-PN-O3	-2.21	101.29	107.27
3	A	1347	NAD	C5A-C6A-N6A	-2.16	117.94	123.29
3	B	1347	NAD	O4B-C1B-N9A	2.13	112.18	108.09
3	A	1347	NAD	O4B-C1B-N9A	-2.13	104.00	108.09
3	B	1347	NAD	O2N-PN-O1N	2.09	122.17	112.44
3	B	1347	NAD	C5D-C4D-C3D	-2.09	107.69	115.21
3	D	1346	NAD	C5D-C4D-C3D	-2.00	108.01	115.21

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1347	NAD	C5B-O5B-PA-O1A
3	A	1347	NAD	C5B-O5B-PA-O2A
3	A	1347	NAD	C5B-O5B-PA-O3
3	A	1347	NAD	PN-O3-PA-O5B
3	B	1347	NAD	C5B-O5B-PA-O1A
3	B	1347	NAD	C5D-O5D-PN-O2N
3	B	1347	NAD	O4D-C1D-N1N-C6N
3	C	1346	NAD	C5B-O5B-PA-O2A
3	C	1346	NAD	C5B-O5B-PA-O3
3	C	1346	NAD	O4B-C4B-C5B-O5B
3	C	1346	NAD	C5D-O5D-PN-O3
3	C	1346	NAD	C5D-O5D-PN-O1N
3	C	1346	NAD	C5D-O5D-PN-O2N
3	D	1346	NAD	C3B-C4B-C5B-O5B
3	D	1346	NAD	C5D-O5D-PN-O3
3	D	1346	NAD	C5D-O5D-PN-O1N
3	D	1346	NAD	C5D-O5D-PN-O2N
3	D	1346	NAD	O4D-C1D-N1N-C6N
3	B	1347	NAD	C3D-C4D-C5D-O5D
3	C	1346	NAD	C3B-C4B-C5B-O5B
3	D	1346	NAD	O4D-C4D-C5D-O5D
3	D	1346	NAD	C3D-C4D-C5D-O5D
3	D	1346	NAD	O4B-C4B-C5B-O5B
3	B	1347	NAD	C3B-C4B-C5B-O5B
3	A	1347	NAD	C3B-C4B-C5B-O5B
3	B	1347	NAD	O4B-C4B-C5B-O5B
3	A	1347	NAD	O4B-C4B-C5B-O5B
3	B	1347	NAD	O4D-C4D-C5D-O5D
3	C	1346	NAD	PN-O3-PA-O5B
3	C	1346	NAD	PA-O3-PN-O5D

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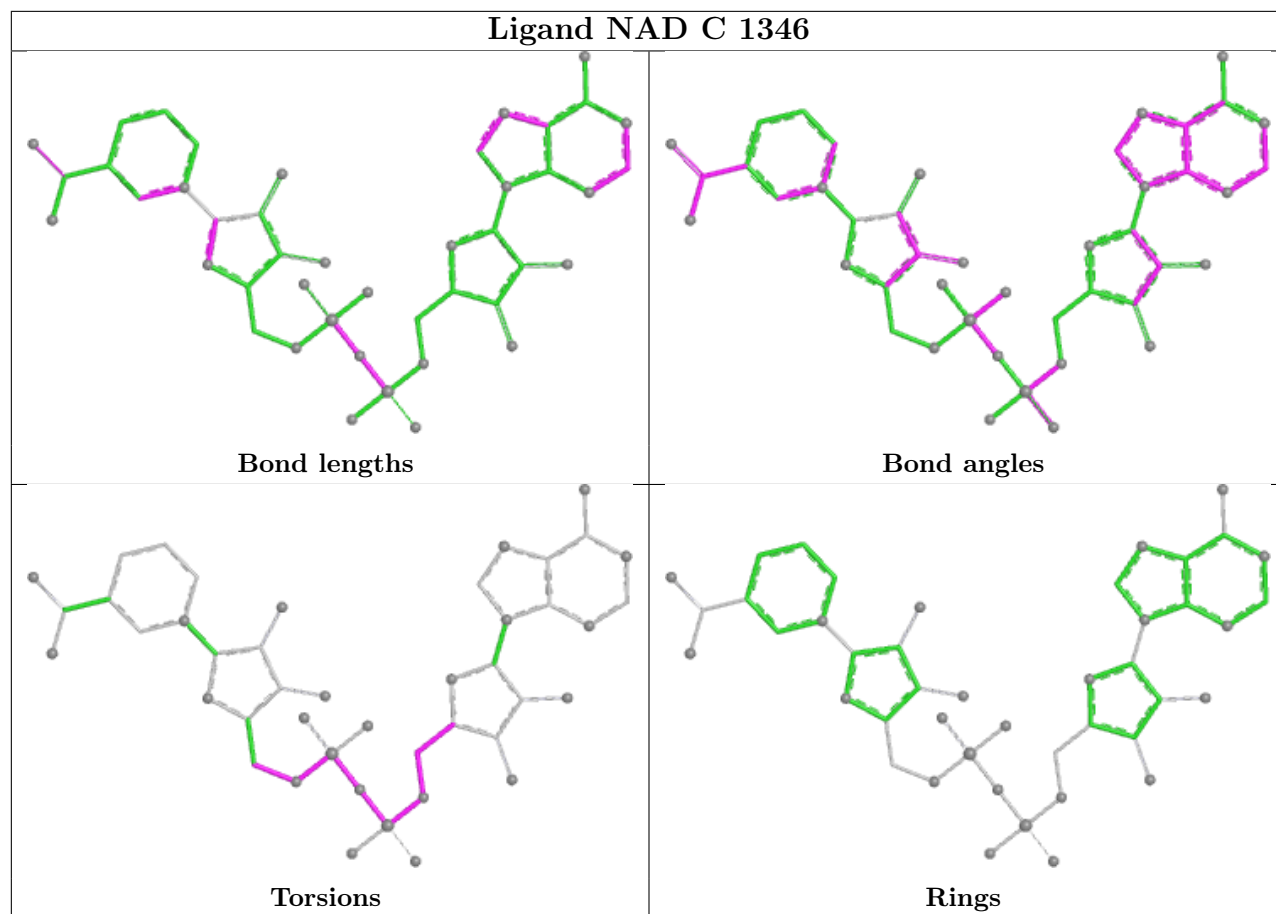
Mol	Chain	Res	Type	Atoms
3	A	1347	NAD	C2B-C1B-N9A-C8A
3	B	1347	NAD	C5B-O5B-PA-O2A
3	B	1347	NAD	C5B-O5B-PA-O3
3	D	1346	NAD	C5B-O5B-PA-O1A
3	A	1347	NAD	C4B-C5B-O5B-PA
3	C	1346	NAD	C4D-C5D-O5D-PN
3	D	1346	NAD	C2B-C1B-N9A-C8A
3	D	1346	NAD	C4B-C5B-O5B-PA
3	B	1347	NAD	O4D-C1D-N1N-C2N
3	D	1346	NAD	O4D-C1D-N1N-C2N
3	C	1346	NAD	C4B-C5B-O5B-PA
3	D	1346	NAD	C4D-C5D-O5D-PN
3	C	1346	NAD	PN-O3-PA-O2A
3	A	1347	NAD	O4B-C1B-N9A-C8A
3	B	1347	NAD	PA-O3-PN-O2N
3	C	1346	NAD	PN-O3-PA-O1A

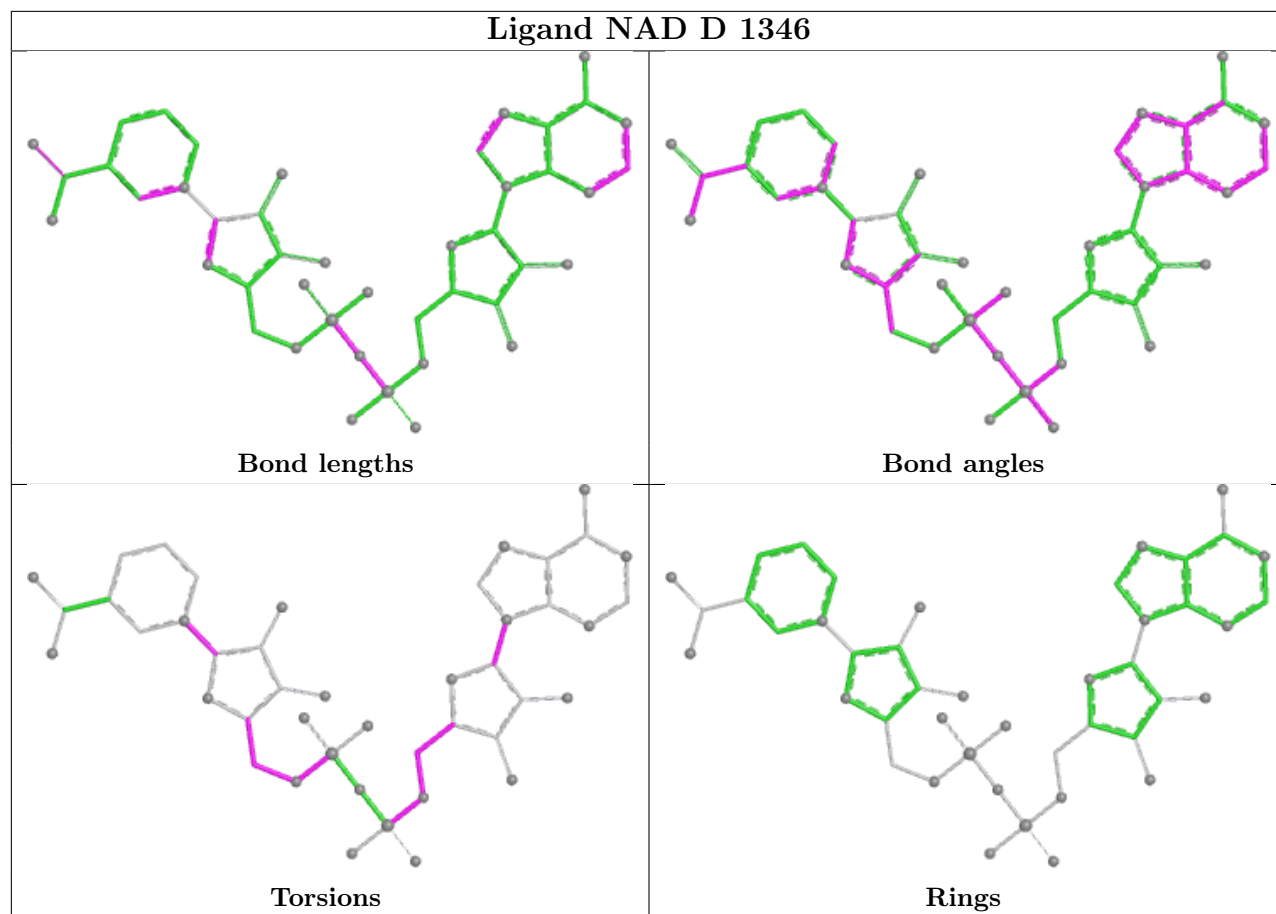
There are no ring outliers.

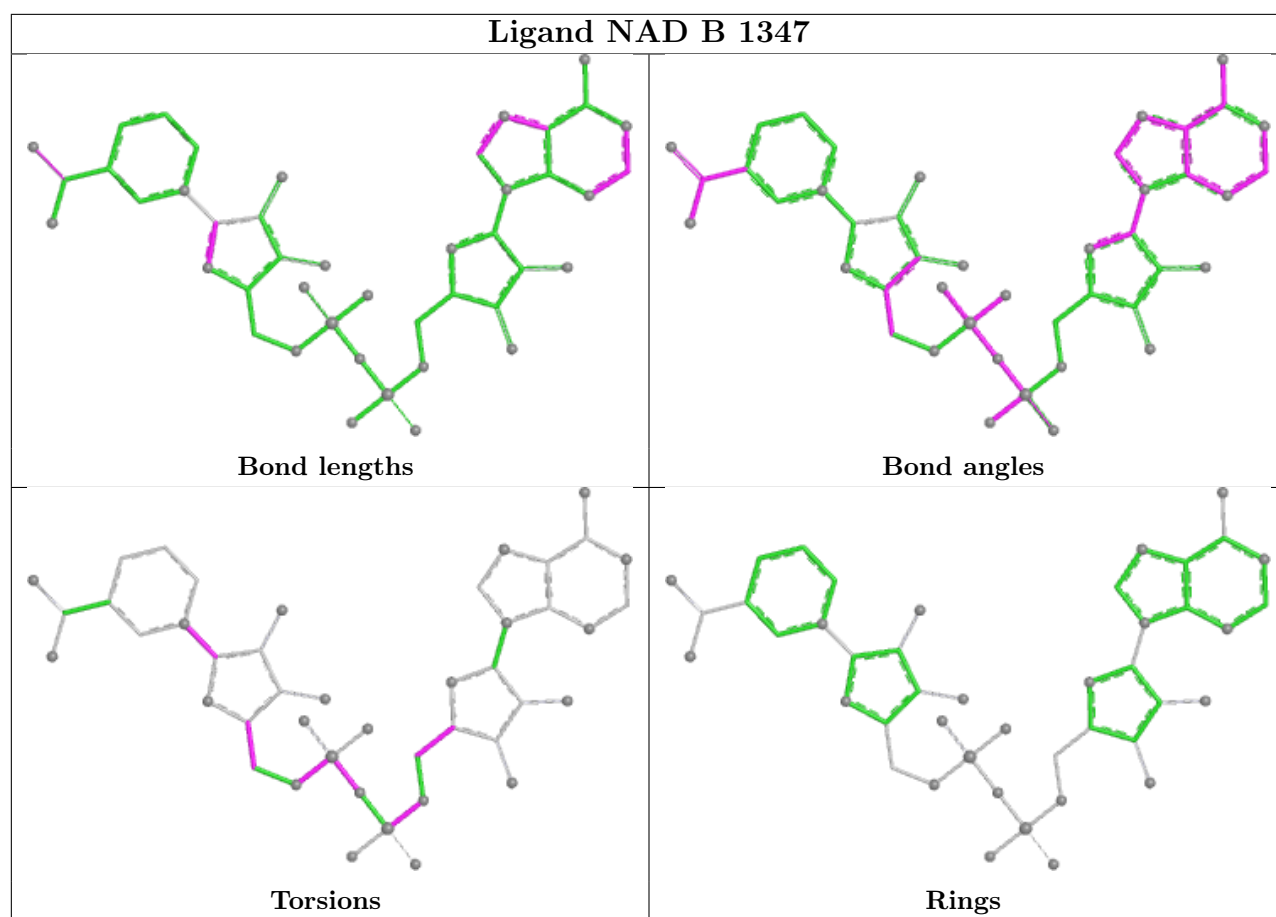
5 monomers are involved in 20 short contacts:

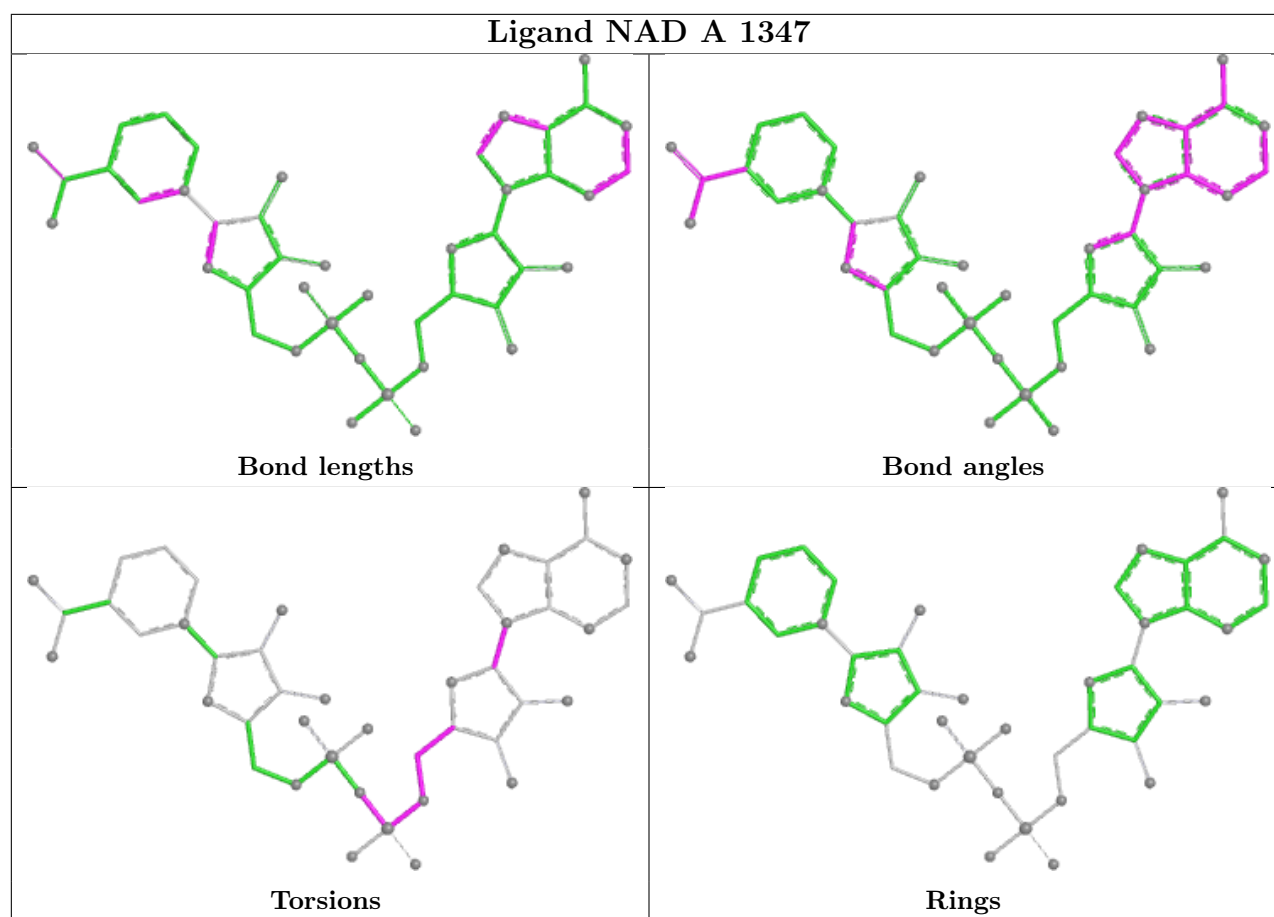
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1346	NAD	2	0
3	D	1346	NAD	9	0
3	B	1347	NAD	4	0
3	A	1347	NAD	4	0
4	B	1348	SO4	1	0

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	346/348 (99%)	-1.62	0 100 100	8, 20, 38, 57	5 (1%)
1	B	345/348 (99%)	-1.59	0 100 100	7, 21, 42, 52	3 (0%)
1	C	344/348 (98%)	-1.69	0 100 100	6, 17, 31, 39	7 (2%)
2	D	345/348 (99%)	-1.68	0 100 100	7, 17, 30, 42	7 (2%)
All	All	1380/1392 (99%)	-1.64	0 100 100	6, 19, 37, 57	22 (1%)

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
4	SO4	C	1347	5/5	0.98	0.04	60,61,61,62	0
3	NAD	B	1347	44/44	0.99	0.04	10,14,17,19	44
3	NAD	C	1346	44/44	0.99	0.05	16,23,25,26	44
3	NAD	D	1346	44/44	0.99	0.06	19,27,30,31	44

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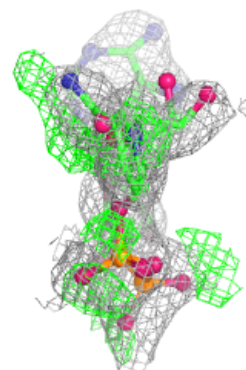
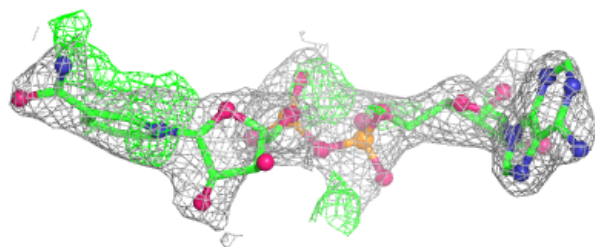
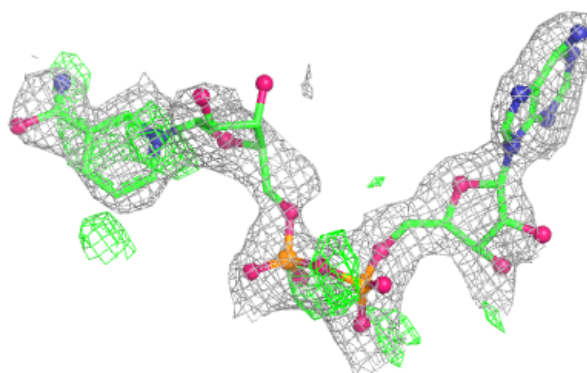
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1348	5/5	0.99	0.04	51,52,53,54	0
4	SO4	B	1348	5/5	0.99	0.04	53,53,55,56	0
3	NAD	A	1347	44/44	0.99	0.06	12,21,22,24	44
4	SO4	D	1347	5/5	0.99	0.04	61,62,63,63	0

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.

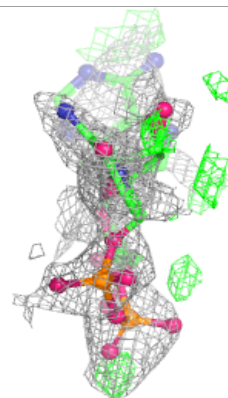
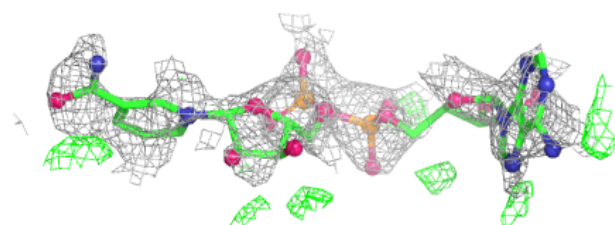
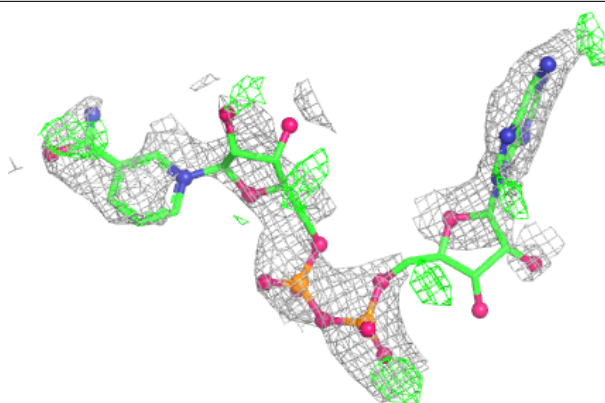
Electron density around NAD B 1347:

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

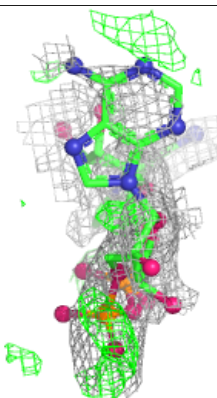
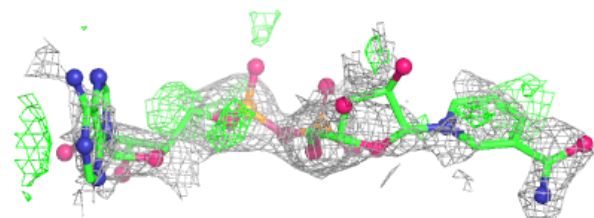
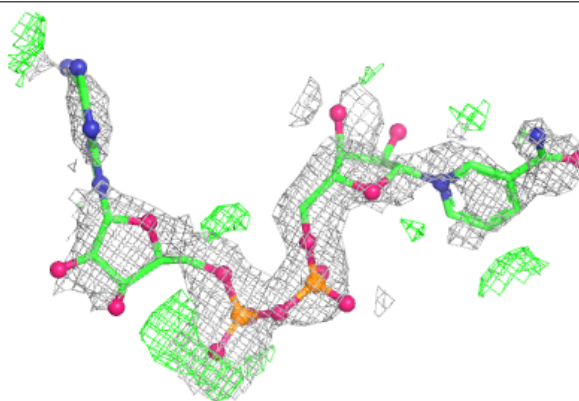


Electron density around NAD C 1346:

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

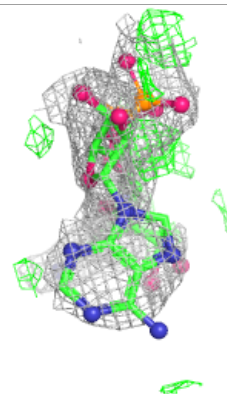
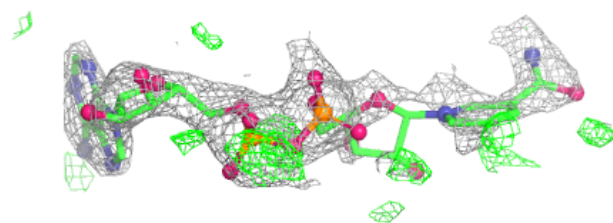
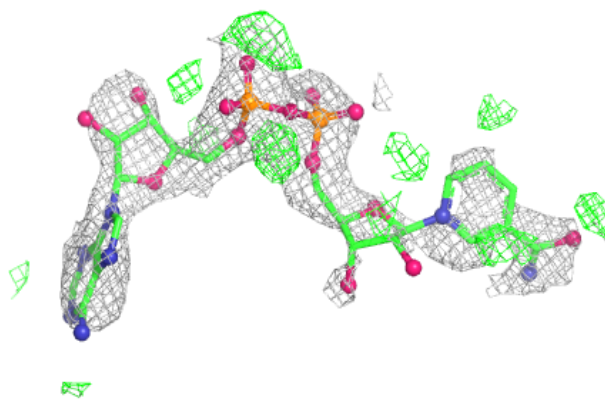
**Electron density around NAD D 1346:**

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



Electron density around NAD A 1347:

$2mF_o-DF_c$ (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.