WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2023 – 12:39 PM EDT

PDB ID	:	1GD1
Title	:	STRUCTURE OF HOLO-GLYCERALDEHYDE-3-PHOSPHATE DE-HYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS AT 1.8 ANGSTROMS RESOLUTION
Authors	:	Skarzynski, T.; Moody, P.C.E.; Wonacott, A.J.
Deposited on	:	1987-06-22
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

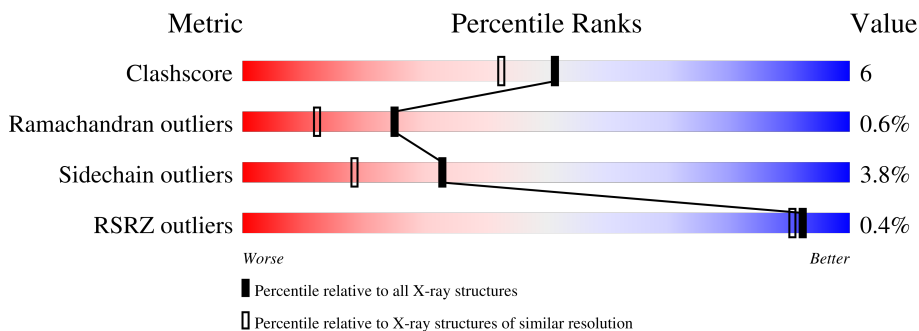|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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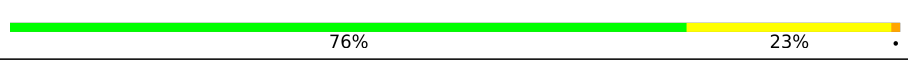*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.6%
Sidechain outliers		3.8%
RSRZ outliers		0.4%

Worse ... *Better*

■ Percentile relative to all X-ray structures

❙ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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.

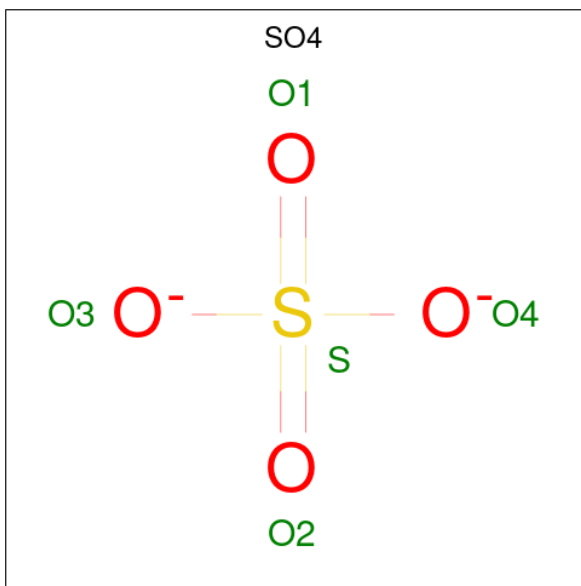| Mol	Chain	Length	Quality of chain
1	O	334	76% 23% •
1	P	334	78% 19% •
1	Q	334	.% 75% 23% • •
1	R	334	.% 76% 21% • •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10984 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 HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHY-DROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			
1	P	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			
1	Q	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			
1	R	334	Total	C	N	O	S	0	0	0
			2525	1582	445	489	9			

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total 5	O 4	S 1	0	0
2	P	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0
2	R	1	Total 5	O 4	S 1	0	0
2	R	1	Total 5	O 4	S 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
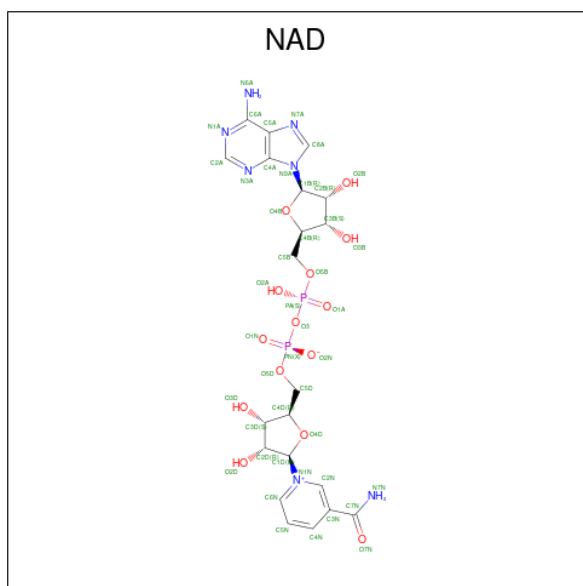
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	P	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	R	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	176	Total 176	O 176	0	0
4	P	162	Total 162	O 162	0	0
4	Q	166	Total 166	O 166	0	0
4	R	164	Total 164	O 164	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: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE
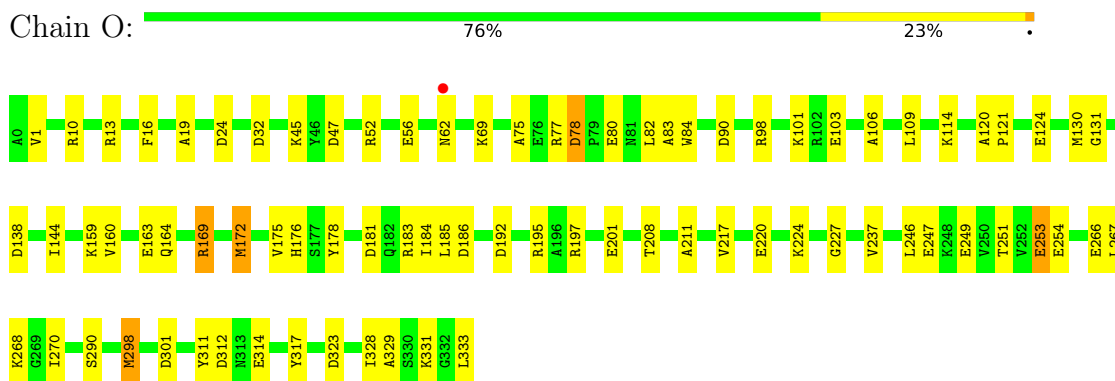
Chain O:

• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain P:

• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain Q:

G265 E266 I270 Y273 R281 D282 Y283 S290 M298 D301 V305 Y311 D312 R320 D323 I328 L333

• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain R:

%

76%   21%

A0 V1 R10 R13 R17 D24 I25 D32 K45 Y46 R52 L53 D54 A55 E56 N60 G61 N62 N63 L64 V65 V73 K74 A75 E76 R77 D78 P79 L82 V93 R98 R102 E103 D104 K107 E110 K122A N123 C149 K159 Q164

F165 G166 R169 G170 M171 M172 T173 Y178 D181 Q182 R183 D186 K191 R194 R195 A196 R197 A198 T208 A211 L218 P219 E220 L225 N226 G227 M230 R231 P235 N236 V237 V240 E245 L246 E247 K248 K260 E264 G265 E266 E276 P277 L278

S289 D293 V308 T315 H319 R320 A329 L333
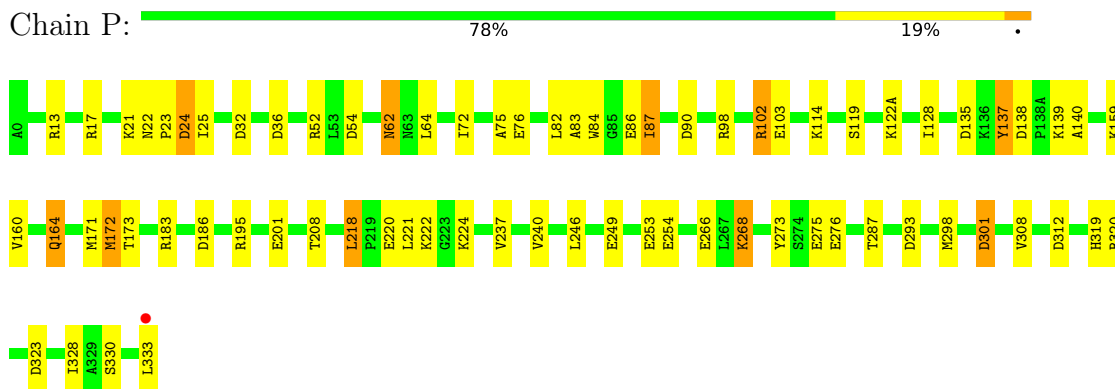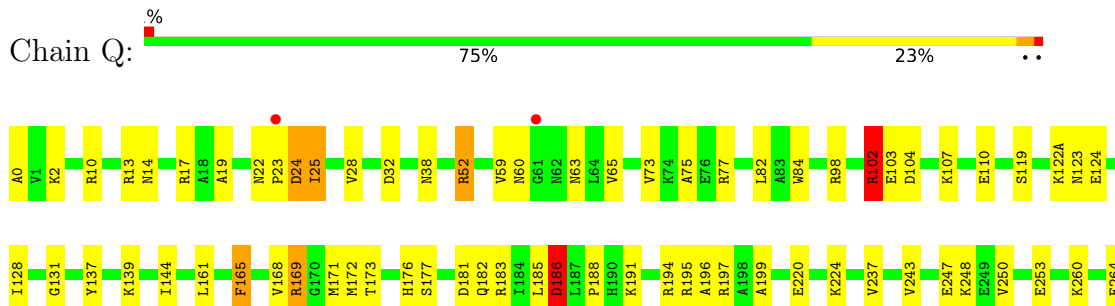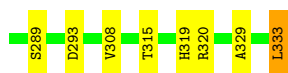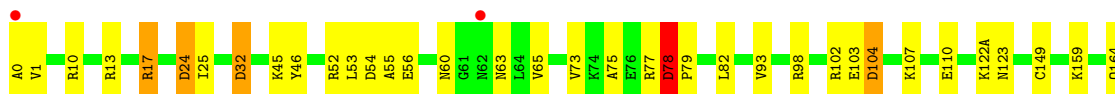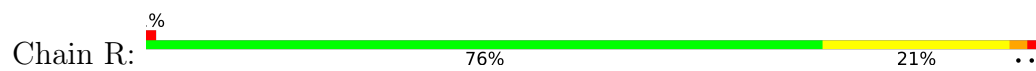
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.44Å 124.10Å 82.54Å 90.00° 108.98° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80 18.81 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 80.1 (18.81-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.137 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10984	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	O	1.06	1/2561 (0.0%)	1.83	54/3474 (1.6%)
1	P	1.09	0/2561	1.76	42/3474 (1.2%)
1	Q	1.07	0/2561	1.85	59/3474 (1.7%)
1	R	1.07	2/2561 (0.1%)	1.81	43/3474 (1.2%)
All	All	1.07	3/10244 (0.0%)	1.81	198/13896 (1.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	178	TYR	CE1-CZ	5.18	1.45	1.38
1	R	78	ASP	CG-OD2	5.14	1.37	1.25
1	R	289	SER	CA-CB	5.06	1.60	1.52

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	266	GLU	CA-CB-CG	18.21	153.47	113.40
1	R	98	ARG	NE-CZ-NH2	-17.60	111.50	120.30
1	Q	98	ARG	NE-CZ-NH2	-17.55	111.52	120.30
1	O	98	ARG	NE-CZ-NH2	-17.54	111.53	120.30
1	P	98	ARG	NE-CZ-NH2	-17.54	111.53	120.30
1	O	10	ARG	NE-CZ-NH1	17.12	128.86	120.30
1	R	98	ARG	NE-CZ-NH1	16.13	128.36	120.30
1	O	98	ARG	NE-CZ-NH1	16.09	128.34	120.30
1	P	98	ARG	NE-CZ-NH1	16.07	128.34	120.30
1	Q	98	ARG	NE-CZ-NH1	16.01	128.31	120.30
1	R	10	ARG	NE-CZ-NH1	15.43	128.01	120.30
1	R	183	ARG	NE-CZ-NH1	14.46	127.53	120.30
1	Q	13	ARG	NE-CZ-NH2	12.43	126.52	120.30
1	Q	10	ARG	NE-CZ-NH1	11.82	126.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	320	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	O	197	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	R	17	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	O	197	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	Q	161	LEU	CB-CG-CD2	10.68	129.15	111.00
1	P	102	ARG	NE-CZ-NH1	-10.67	114.96	120.30
1	Q	312	ASP	CB-CG-OD1	10.58	127.82	118.30
1	P	135	ASP	CB-CG-OD1	10.54	127.78	118.30
1	P	312	ASP	CB-CG-OD1	10.34	127.61	118.30
1	O	10	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	O	195	ARG	NE-CZ-NH2	10.26	125.43	120.30
1	R	266	GLU	CA-CB-CG	9.97	135.33	113.40
1	P	301	ASP	CB-CG-OD1	9.84	127.16	118.30
1	Q	323	ASP	CB-CG-OD1	9.78	127.10	118.30
1	Q	183	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	R	231	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	R	231	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	O	183	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	P	301	ASP	CB-CG-OD2	-9.33	109.90	118.30
1	Q	197	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	Q	13	ARG	CD-NE-CZ	9.17	136.44	123.60
1	P	13	ARG	CD-NE-CZ	9.01	136.22	123.60
1	R	264	GLU	OE1-CD-OE2	8.96	134.05	123.30
1	Q	194	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	P	13	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	R	10	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	Q	52	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	O	169	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	P	36	ASP	CB-CG-OD1	8.46	125.91	118.30
1	Q	281	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	P	201	GLU	OE1-CD-OE2	8.44	133.43	123.30
1	Q	104	ASP	CB-CG-OD1	8.37	125.83	118.30
1	P	266	GLU	CB-CG-CD	8.24	136.44	114.20
1	Q	183	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	Q	17	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	P	17	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	O	201	GLU	OE1-CD-OE2	8.11	133.04	123.30
1	O	47	ASP	O-C-N	8.02	135.54	122.70
1	R	104	ASP	CB-CG-OD1	8.00	125.50	118.30
1	R	32	ASP	CB-CG-OD1	7.98	125.48	118.30
1	O	312	ASP	CB-CG-OD1	7.91	125.42	118.30
1	R	13	ARG	CD-NE-CZ	7.70	134.38	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	301	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	P	17	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	P	266	GLU	OE1-CD-OE2	-7.49	114.31	123.30
1	O	138	ASP	CB-CG-OD1	7.47	125.03	118.30
1	O	323	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	Q	102	ARG	CB-CA-C	7.42	125.25	110.40
1	Q	323	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	O	77	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	Q	311	TYR	CB-CG-CD2	7.38	125.43	121.00
1	R	102	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	R	78	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	Q	169	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	Q	281	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	R	194	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	O	301	ASP	CB-CG-OD1	7.14	124.73	118.30
1	O	195	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	R	181	ASP	CB-CG-OD1	7.04	124.64	118.30
1	R	52	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	Q	77	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	P	173	THR	N-CA-CB	6.94	123.48	110.30
1	Q	283	TYR	CB-CG-CD1	-6.89	116.86	121.00
1	P	17	ARG	CD-NE-CZ	6.88	133.23	123.60
1	O	311	TYR	CB-CG-CD2	6.84	125.10	121.00
1	Q	181	ASP	CB-CG-OD1	6.83	124.45	118.30
1	R	186	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	O	24	ASP	CB-CG-OD1	6.76	124.38	118.30
1	P	64	LEU	CA-CB-CG	6.73	130.77	115.30
1	Q	124	GLU	OE1-CD-OE2	-6.69	115.27	123.30
1	Q	197	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	O	253	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	R	54	ASP	CB-CG-OD1	6.62	124.25	118.30
1	O	78	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	P	140	ALA	N-CA-CB	-6.54	100.94	110.10
1	P	54	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	O	169	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	O	323	ASP	CB-CG-OD1	6.46	124.11	118.30
1	R	173	THR	N-CA-CB	6.30	122.27	110.30
1	O	77	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	R	198	ALA	CB-CA-C	6.28	119.52	110.10
1	P	137	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	O	290	SER	N-CA-CB	-6.24	101.14	110.50
1	O	176	HIS	N-CA-CB	-6.23	99.38	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	77	ARG	CA-CB-CG	6.23	127.10	113.40
1	R	293	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	P	13	ARG	NH1-CZ-NH2	-6.22	112.56	119.40
1	P	320	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	R	24	ASP	CB-CG-OD1	6.19	123.87	118.30
1	Q	195	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	P	24	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	Q	161	LEU	CA-CB-CG	6.17	129.49	115.30
1	Q	290	SER	N-CA-CB	-6.14	101.28	110.50
1	Q	266	GLU	CG-CD-OE1	6.12	130.53	118.30
1	Q	173	THR	N-CA-CB	6.09	121.87	110.30
1	R	93	VAL	O-C-N	6.09	132.44	122.70
1	O	80	GLU	OE1-CD-OE2	6.06	130.57	123.30
1	P	195	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	R	169	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	Q	52	ARG	CD-NE-CZ	6.01	132.01	123.60
1	O	47	ASP	CA-C-N	-5.99	104.03	117.20
1	Q	312	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	R	46	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	O	298	MET	CA-CB-CG	5.97	123.44	113.30
1	R	230	MET	CA-CB-CG	-5.97	103.16	113.30
1	O	314	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	P	276	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	O	124	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	P	273	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	Q	102	ARG	N-CA-CB	-5.92	99.94	110.60
1	R	149	CYS	CB-CA-C	5.92	122.24	110.40
1	R	264	GLU	CG-CD-OE2	-5.91	106.49	118.30
1	Q	102	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	Q	281	ARG	N-CA-CB	5.90	121.22	110.60
1	O	314	GLU	CG-CD-OE2	-5.86	106.57	118.30
1	P	102	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	Q	24	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	Q	298	MET	N-CA-CB	-5.82	100.13	110.60
1	P	138	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	Q	186	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	P	293	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	R	56	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	O	52	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	O	130	MET	CG-SD-CE	-5.63	91.19	100.20
1	R	245	GLU	OE1-CD-OE2	5.63	130.05	123.30
1	R	178	TYR	CB-CG-CD2	-5.62	117.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	80	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	Q	176	HIS	N-CA-CB	-5.58	100.55	110.60
1	O	90	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	O	317	TYR	CG-CD2-CE2	-5.58	116.84	121.30
1	O	13	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	P	183	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	Q	52	ARG	CG-CD-NE	5.57	123.50	111.80
1	R	32	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	P	195	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	P	298	MET	N-CA-CB	-5.52	100.67	110.60
1	O	333	LEU	CA-CB-CG	5.52	127.99	115.30
1	Q	17	ARG	CD-NE-CZ	5.51	131.31	123.60
1	R	247	GLU	CB-CG-CD	5.49	129.03	114.20
1	Q	171	MET	N-CA-CB	5.48	120.46	110.60
1	Q	250	VAL	O-C-N	5.47	131.45	122.70
1	O	178	TYR	CD1-CE1-CZ	-5.46	114.89	119.80
1	P	218	LEU	CA-C-O	5.42	131.49	120.10
1	R	56	GLU	CG-CD-OE2	-5.42	107.46	118.30
1	P	275	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	Q	110	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	Q	77	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	R	13	ARG	O-C-N	5.34	131.25	122.70
1	R	104	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	P	52	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	P	266	GLU	CG-CD-OE1	5.28	128.85	118.30
1	Q	199	ALA	CB-CA-C	-5.25	102.22	110.10
1	Q	253	GLU	OE1-CD-OE2	-5.24	117.02	123.30
1	O	13	ARG	CD-NE-CZ	5.23	130.92	123.60
1	P	253	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	O	178	TYR	CG-CD1-CE1	5.21	125.47	121.30
1	Q	195	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	Q	110	GLU	CB-CG-CD	5.20	128.25	114.20
1	R	55	ALA	O-C-N	5.20	131.03	122.70
1	O	138	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	P	323	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	R	77	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	O	192	ASP	CB-CG-OD1	5.19	122.97	118.30
1	Q	266	GLU	CB-CG-CD	5.18	128.19	114.20
1	R	197	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	O	78	ASP	OD1-CG-OD2	5.16	133.11	123.30
1	Q	14	ASN	CB-CA-C	5.16	120.72	110.40
1	P	102	ARG	CG-CD-NE	-5.15	100.98	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	130	MET	N-CA-CB	-5.12	101.38	110.60
1	Q	194	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	R	183	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	O	298	MET	CB-CA-C	5.09	120.57	110.40
1	O	181	ASP	CB-CG-OD1	5.08	122.88	118.30
1	P	254	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	O	175	VAL	N-CA-C	-5.07	97.30	111.00
1	O	217	VAL	C-N-CA	5.06	134.36	121.70
1	Q	177	SER	O-C-N	5.06	130.79	122.70
1	O	249	GLU	CA-CB-CG	5.06	124.53	113.40
1	O	101	LYS	CA-CB-CG	5.05	124.52	113.40
1	O	181	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	O	253	GLU	CG-CD-OE1	5.03	128.36	118.30
1	Q	320	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	Q	273	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	P	287	THR	CA-CB-CG2	5.00	119.41	112.40

There are no chirality outliers.

There are no planarity outliers.

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	O	2525	0	2572	24	0
1	P	2525	0	2572	24	0
1	Q	2525	0	2572	38	0
1	R	2525	0	2572	32	0
2	O	10	0	0	0	0
2	P	10	0	0	0	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	O	44	0	26	0	0
3	P	44	0	26	1	0
3	Q	44	0	26	1	0
3	R	44	0	26	0	0
4	O	176	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	162	0	0	3	0
4	Q	166	0	0	2	0
4	R	164	0	0	3	0
All	All	10984	0	10392	116	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 6.

All (116) 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:Q:102:ARG:HH11	1:Q:102:ARG:HG3	1.38	0.88
1:Q:220:GLU:H	1:Q:220:GLU:CD	1.89	0.74
1:O:16:PHE:HA	4:O:434:HOH:O	1.91	0.69
1:Q:102:ARG:HH11	1:Q:102:ARG:CG	2.06	0.69
1:R:172:MET:CE	1:R:208:THR:HG21	2.24	0.67
1:Q:102:ARG:HG3	1:Q:102:ARG:NH1	2.07	0.67
1:Q:102:ARG:CG	1:Q:102:ARG:NH1	2.58	0.66
1:P:76:GLU:OE2	4:P:425:HOH:O	2.14	0.65
1:Q:60:ASN:HB2	1:Q:65:VAL:CG2	2.28	0.64
1:P:172:MET:CE	1:P:208:THR:HG21	2.29	0.63
1:R:329:ALA:HA	1:R:333:LEU:HD22	1.82	0.61
1:O:144:ILE:HD13	1:O:328:ILE:HD11	1.82	0.61
1:Q:168:VAL:CG2	1:Q:247:GLU:HG3	2.32	0.60
1:R:0:ALA:HB3	1:R:24:ASP:O	2.02	0.59
1:R:165:PHE:HA	1:R:248:LYS:HD2	1.84	0.59
1:R:122(A):LYS:O	1:R:123:ASN:HB2	2.01	0.59
1:Q:144:ILE:HD13	1:Q:328:ILE:HD11	1.84	0.58
1:P:83:ALA:HB1	1:P:86:GLU:OE2	2.03	0.58
1:Q:22:ASN:OD1	1:Q:24:ASP:HB2	2.04	0.58
1:Q:0:ALA:HB3	1:Q:24:ASP:O	2.05	0.57
1:O:266:GLU:HG3	1:O:267:LEU:HG	1.85	0.56
1:Q:128:ILE:HD11	1:Q:137:TYR:HB2	1.85	0.56
1:Q:191:LYS:HG2	4:Q:432:HOH:O	2.05	0.56
1:P:114:LYS:HD2	1:P:333:LEU:HG	1.88	0.55
1:O:19:ALA:HB3	4:O:434:HOH:O	2.07	0.55
1:R:107:LYS:HA	1:R:110:GLU:HG3	1.89	0.55
1:Q:60:ASN:HB2	1:Q:65:VAL:HG23	1.89	0.54
1:O:172:MET:CE	1:O:208:THR:HG21	2.38	0.54
1:Q:19:ALA:CB	1:Q:25:ILE:HD11	2.38	0.54
1:O:251:THR:OG1	1:O:254:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:220:GLU:H	1:R:220:GLU:CD	2.11	0.53
1:Q:144:ILE:HD13	1:Q:328:ILE:CD1	2.37	0.53
1:P:159:LYS:HB2	1:P:218:LEU:HD11	1.91	0.53
1:R:191:LYS:HG2	4:R:429:HOH:O	2.08	0.53
1:O:172:MET:HG3	1:O:227:GLY:HA3	1.91	0.52
1:Q:19:ALA:HB1	1:Q:25:ILE:HD11	1.90	0.52
1:R:172:MET:HE1	1:R:208:THR:HG21	1.90	0.52
1:P:224:LYS:NZ	4:P:464:HOH:O	2.28	0.52
1:Q:165:PHE:O	1:Q:248:LYS:HG3	2.11	0.51
1:O:131:GLY:HA3	1:O:270:ILE:HD13	1.93	0.51
1:P:240:VAL:O	1:P:308:VAL:HA	2.12	0.50
1:O:45:LYS:HG2	4:O:401:HOH:O	2.11	0.50
1:O:144:ILE:HD13	1:O:328:ILE:CD1	2.42	0.49
1:O:298:MET:HG2	1:P:171:MET:CE	2.42	0.49
1:R:172:MET:HG2	1:R:211:ALA:HB2	1.95	0.49
1:P:128:ILE:HD11	1:P:137:TYR:HB2	1.93	0.49
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.48	0.49
1:R:78:ASP:HB2	4:R:433:HOH:O	2.13	0.48
1:P:90:ASP:OD1	1:P:114:LYS:HE3	2.14	0.48
1:P:160:VAL:O	1:P:164:GLN:HB2	2.13	0.48
1:O:224:LYS:NZ	4:O:471:HOH:O	2.41	0.48
1:R:186:ASP:HA	1:R:196:ALA:O	2.14	0.48
1:R:1:VAL:CG1	1:R:25:ILE:HG22	2.44	0.47
1:O:169:ARG:HD3	1:P:301:ASP:HB2	1.96	0.47
1:R:60:ASN:HB2	1:R:65:VAL:CG2	2.45	0.47
1:R:164:GLN:NE2	4:R:444:HOH:O	2.47	0.47
1:Q:182:GLN:HB3	4:Q:374:HOH:O	2.14	0.47
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.50	0.46
1:R:45:LYS:HB2	1:R:45:LYS:HE3	1.69	0.46
1:R:79:PRO:HA	1:R:82:LEU:HD12	1.98	0.46
1:O:1:VAL:HG21	1:O:329:ALA:HB1	1.98	0.46
1:P:21:LYS:HE2	1:P:319:HIS:HE1	1.81	0.46
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.51	0.45
1:P:102:ARG:HG3	1:P:102:ARG:NH1	2.31	0.45
1:R:172:MET:HE2	1:R:208:THR:HG21	1.97	0.45
1:Q:333:LEU:HD12	1:Q:333:LEU:HA	1.84	0.45
1:P:32:ASP:O	1:P:75:ALA:HA	2.17	0.45
1:R:103:GLU:HG3	1:R:104:ASP:N	2.32	0.45
1:O:106:ALA:O	1:O:109:LEU:HB2	2.16	0.45
1:P:72:ILE:HD13	1:P:87:ILE:HG21	1.99	0.44
1:R:172:MET:HG3	1:R:227:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:139:LYS:HD2	1:P:139:LYS:HA	1.80	0.43
1:Q:22:ASN:OD1	1:Q:23:PRO:HD2	2.19	0.43
1:O:159:LYS:O	1:O:163:GLU:HG3	2.19	0.43
1:Q:38:ASN:ND2	1:Q:59:VAL:HG11	2.33	0.43
1:Q:260:LYS:NZ	1:Q:264:GLU:OE2	2.51	0.43
1:R:166:GLY:HA3	1:R:247:GLU:HG3	2.01	0.43
1:P:62:ASN:HD22	1:P:62:ASN:HA	1.59	0.43
1:Q:60:ASN:HB2	1:Q:65:VAL:HG21	1.98	0.43
1:O:82:LEU:O	1:O:83:ALA:HB3	2.19	0.43
1:R:17:ARG:HG2	1:R:53:LEU:CD1	2.48	0.43
1:P:328:ILE:HD13	1:P:328:ILE:HG21	1.78	0.42
1:Q:38:ASN:HD21	1:Q:59:VAL:HG11	1.83	0.42
1:O:184:ILE:HG22	1:O:185:LEU:HG	2.01	0.42
1:O:172:MET:HG2	1:O:211:ALA:HB2	2.01	0.42
1:R:17:ARG:HG2	1:R:53:LEU:HD13	2.01	0.42
1:Q:119:SER:O	3:Q:336:NAD:H6N	2.20	0.42
1:Q:186:ASP:HA	1:Q:196:ALA:O	2.19	0.42
1:R:276:GLU:HB2	1:R:278:LEU:HG	2.00	0.42
1:R:63:ASN:ND2	1:R:73:VAL:H	2.18	0.42
1:O:120:ALA:HB1	1:O:121:PRO:CD	2.50	0.42
1:Q:139:LYS:HA	1:Q:139:LYS:HD2	1.92	0.42
1:R:315:THR:O	1:R:319:HIS:HD2	2.02	0.42
1:Q:243:VAL:HA	1:Q:305:VAL:O	2.20	0.41
1:O:32:ASP:O	1:O:75:ALA:HA	2.19	0.41
1:P:221:LEU:O	1:P:222:LYS:C	2.58	0.41
1:Q:32:ASP:O	1:Q:75:ALA:HA	2.19	0.41
1:Q:169:ARG:HA	1:Q:224:LYS:O	2.20	0.41
1:R:159:LYS:HB2	1:R:218:LEU:HD11	2.01	0.41
1:O:114:LYS:HD2	4:O:485:HOH:O	2.21	0.41
4:P:368:HOH:O	1:Q:188:PRO:HD3	2.19	0.41
1:Q:63:ASN:ND2	1:Q:73:VAL:H	2.18	0.41
1:Q:102:ARG:HB3	1:Q:123:ASN:HB2	2.03	0.41
1:Q:185:LEU:O	1:Q:186:ASP:C	2.59	0.41
1:Q:131:GLY:HA3	1:Q:270:ILE:HD13	2.02	0.41
1:R:170:GLY:O	1:R:225:LEU:HA	2.21	0.41
1:R:32:ASP:O	1:R:75:ALA:HA	2.21	0.41
1:R:60:ASN:HB2	1:R:65:VAL:HG21	2.01	0.41
1:R:79:PRO:HA	1:R:82:LEU:CD1	2.51	0.41
1:Q:168:VAL:HG22	1:Q:247:GLU:HG3	2.03	0.41
1:Q:2:LYS:HE2	1:Q:28:VAL:HG11	2.01	0.40
1:P:119:SER:O	3:P:336:NAD:H1D	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:160:VAL:O	1:O:164:GLN:HB2	2.21	0.40
1:P:268:LYS:HE3	1:P:268:LYS:HB2	1.88	0.40
1:R:240:VAL:O	1:R:308:VAL:HA	2.21	0.40
1:P:22:ASN:OD1	1:P:24:ASP:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	O	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	25	12
1	P	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	25	12
1	Q	332/334 (99%)	316 (95%)	14 (4%)	2 (1%)	25	12
1	R	332/334 (99%)	318 (96%)	12 (4%)	2 (1%)	25	12
All	All	1328/1336 (99%)	1264 (95%)	56 (4%)	8 (1%)	25	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	186	ASP
1	O	237	VAL
1	P	237	VAL
1	Q	186	ASP
1	Q	237	VAL
1	R	186	ASP
1	R	237	VAL
1	O	186	ASP

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	O	272/272 (100%)	260 (96%)	12 (4%)	28	14
1	P	272/272 (100%)	259 (95%)	13 (5%)	25	11
1	Q	272/272 (100%)	262 (96%)	10 (4%)	34	19
1	R	272/272 (100%)	266 (98%)	6 (2%)	52	39
All	All	1088/1088 (100%)	1047 (96%)	41 (4%)	33	18

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	56	GLU
1	O	62	ASN
1	O	69	LYS
1	O	78	ASP
1	O	103	GLU
1	O	172	MET
1	O	220	GLU
1	O	246	LEU
1	O	247	GLU
1	O	253	GLU
1	O	268	LYS
1	O	331	LYS
1	P	23	PRO
1	P	25	ILE
1	P	62	ASN
1	P	87	ILE
1	P	103	GLU
1	P	122(A)	LYS
1	P	164	GLN
1	P	172	MET
1	P	220	GLU
1	P	246	LEU
1	P	249	GLU
1	P	268	LYS

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Mol	Chain	Res	Type
1	P	330	SER
1	Q	25	ILE
1	Q	52	ARG
1	Q	102	ARG
1	Q	103	GLU
1	Q	107	LYS
1	Q	122(A)	LYS
1	Q	165	PHE
1	Q	172	MET
1	Q	266	GLU
1	Q	333	LEU
1	R	78	ASP
1	R	235	PRO
1	R	246	LEU
1	R	260	LYS
1	R	266	GLU
1	R	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	62	ASN
1	O	63	ASN
1	O	81	ASN
1	O	146	ASN
1	O	152	ASN
1	O	256	ASN
1	P	62	ASN
1	P	63	ASN
1	P	146	ASN
1	P	152	ASN
1	P	256	ASN
1	Q	38	ASN
1	Q	63	ASN
1	Q	152	ASN
1	Q	256	ASN
1	Q	319	HIS
1	R	63	ASN
1	R	146	ASN
1	R	152	ASN
1	R	256	ASN
1	R	319	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\#|Z| > 2$
2	SO4	R	338	-	4,4,4	0.58	0	6,6,6	0.56	0
3	NAD	P	336	-	42,48,48	1.31	6 (14%)	50,73,73	1.72	12 (24%)
3	NAD	Q	336	-	42,48,48	1.42	5 (11%)	50,73,73	1.98	15 (30%)
2	SO4	O	338	-	4,4,4	0.63	0	6,6,6	0.62	0
2	SO4	Q	339	-	4,4,4	1.11	0	6,6,6	0.50	0
2	SO4	O	339	-	4,4,4	1.19	0	6,6,6	0.75	0
2	SO4	Q	338	-	4,4,4	0.79	0	6,6,6	1.21	1 (16%)
3	NAD	O	336	-	42,48,48	1.17	3 (7%)	50,73,73	2.03	12 (24%)
2	SO4	R	339	-	4,4,4	0.85	0	6,6,6	0.60	0
3	NAD	R	336	-	42,48,48	1.18	2 (4%)	50,73,73	2.09	13 (26%)
2	SO4	P	339	-	4,4,4	0.90	0	6,6,6	0.53	0
2	SO4	P	338	-	4,4,4	0.52	0	6,6,6	0.69	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	Q	336	-	-	5/26/62/62	0/5/5/5
3	NAD	P	336	-	-	6/26/62/62	0/5/5/5
3	NAD	R	336	-	-	6/26/62/62	0/5/5/5
3	NAD	O	336	-	-	5/26/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	336	NAD	C3N-C7N	5.31	1.58	1.50
3	P	336	NAD	C3N-C7N	4.70	1.57	1.50
3	R	336	NAD	C3N-C7N	4.63	1.57	1.50
3	O	336	NAD	C3N-C7N	4.04	1.56	1.50
3	Q	336	NAD	O4B-C1B	3.12	1.45	1.41
3	Q	336	NAD	PN-O2N	-2.86	1.41	1.55
3	P	336	NAD	O4B-C1B	2.76	1.44	1.41
3	O	336	NAD	C6N-N1N	2.76	1.42	1.35
3	Q	336	NAD	O4B-C4B	2.61	1.50	1.45
3	P	336	NAD	PN-O2N	-2.51	1.43	1.55
3	Q	336	NAD	C6N-N1N	2.34	1.41	1.35
3	R	336	NAD	C4N-C3N	2.23	1.43	1.39
3	P	336	NAD	C6N-N1N	2.20	1.40	1.35
3	P	336	NAD	C2A-N1A	2.09	1.37	1.33
3	O	336	NAD	O4B-C1B	2.08	1.44	1.41
3	P	336	NAD	PA-O1A	-2.02	1.43	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	336	NAD	O7N-C7N-C3N	-5.85	112.63	119.63
3	R	336	NAD	C5N-C4N-C3N	-5.68	113.62	120.34
3	O	336	NAD	C5N-C6N-N1N	-5.62	112.34	120.40
3	O	336	NAD	C6N-N1N-C2N	4.75	126.31	121.97
3	Q	336	NAD	C2N-C3N-C4N	4.71	123.59	118.26
3	Q	336	NAD	C4N-C3N-C7N	-4.66	108.57	121.04
3	R	336	NAD	C4N-C3N-C7N	-4.53	108.92	121.04
3	R	336	NAD	C6N-C5N-C4N	4.43	125.88	119.44
3	O	336	NAD	C6N-C5N-C4N	4.39	125.82	119.44
3	R	336	NAD	C2N-C3N-C4N	4.22	123.04	118.26
3	O	336	NAD	C4N-C3N-C7N	-4.11	110.04	121.04
3	Q	336	NAD	C5N-C6N-N1N	-4.09	114.53	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	336	NAD	C4N-C3N-C7N	-3.79	110.89	121.04
3	Q	336	NAD	C3N-C2N-N1N	-3.78	116.73	120.43
3	O	336	NAD	C5N-C4N-C3N	-3.72	115.94	120.34
3	O	336	NAD	C3N-C7N-N7N	3.62	122.09	117.75
3	R	336	NAD	C5N-C6N-N1N	-3.52	115.35	120.40
3	P	336	NAD	C5N-C4N-C3N	-3.48	116.22	120.34
3	P	336	NAD	C5N-C6N-N1N	-3.42	115.50	120.40
3	Q	336	NAD	C5N-C4N-C3N	-3.38	116.34	120.34
3	P	336	NAD	C2N-C3N-C4N	3.38	122.09	118.26
3	Q	336	NAD	O7N-C7N-C3N	-3.21	115.80	119.63
3	O	336	NAD	C2N-C3N-C4N	3.18	121.87	118.26
3	Q	336	NAD	C2A-N1A-C6A	3.18	124.19	118.75
3	Q	336	NAD	C6N-N1N-C2N	3.11	124.81	121.97
3	Q	336	NAD	C6N-C5N-C4N	3.11	123.96	119.44
3	O	336	NAD	C3N-C2N-N1N	-2.99	117.50	120.43
3	P	336	NAD	C6N-N1N-C2N	2.99	124.70	121.97
3	O	336	NAD	C2N-C3N-C7N	2.97	128.09	119.46
3	R	336	NAD	N6A-C6A-N1A	2.96	124.73	118.57
3	P	336	NAD	C6N-C5N-C4N	2.91	123.67	119.44
3	R	336	NAD	C2N-C3N-C7N	2.90	127.89	119.46
3	Q	336	NAD	C2N-C3N-C7N	2.88	127.84	119.46
3	R	336	NAD	O7N-C7N-N7N	2.84	126.61	122.58
3	O	336	NAD	C5A-C6A-N6A	2.79	124.60	120.35
3	P	336	NAD	C3N-C2N-N1N	-2.74	117.75	120.43
3	Q	336	NAD	O7N-C7N-N7N	2.72	126.44	122.58
3	R	336	NAD	C4A-C5A-N7A	2.67	112.18	109.40
3	Q	336	NAD	C5A-C6A-N1A	-2.65	114.35	120.35
3	O	336	NAD	O3D-C3D-C4D	-2.64	103.41	111.05
3	Q	336	NAD	N3A-C2A-N1A	-2.61	124.59	128.68
3	P	336	NAD	C2N-C3N-C7N	2.58	126.97	119.46
3	P	336	NAD	C4A-C5A-N7A	2.51	112.02	109.40
3	R	336	NAD	C3N-C7N-N7N	2.51	120.76	117.75
3	O	336	NAD	O7N-C7N-C3N	-2.50	116.64	119.63
3	P	336	NAD	C1B-N9A-C4A	-2.44	122.36	126.64
2	Q	338	SO4	O4-S-O1	2.30	121.34	109.31
3	P	336	NAD	O2A-PA-O5B	-2.28	97.16	107.75
3	P	336	NAD	O4D-C1D-C2D	-2.27	103.61	106.93
3	Q	336	NAD	C5A-C6A-N6A	2.21	123.71	120.35
3	R	336	NAD	C5A-C6A-N1A	-2.11	115.58	120.35
3	Q	336	NAD	O4B-C1B-C2B	-2.08	103.89	106.93
3	R	336	NAD	C3N-C2N-N1N	-2.07	118.40	120.43

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	336	NAD	O4D-C1D-N1N-C2N
3	O	336	NAD	O4D-C1D-N1N-C6N
3	O	336	NAD	C2D-C1D-N1N-C2N
3	O	336	NAD	C2D-C1D-N1N-C6N
3	P	336	NAD	O4D-C1D-N1N-C2N
3	P	336	NAD	O4D-C1D-N1N-C6N
3	P	336	NAD	C2D-C1D-N1N-C2N
3	P	336	NAD	C2D-C1D-N1N-C6N
3	Q	336	NAD	O4D-C1D-N1N-C2N
3	Q	336	NAD	O4D-C1D-N1N-C6N
3	Q	336	NAD	C2D-C1D-N1N-C2N
3	Q	336	NAD	C2D-C1D-N1N-C6N
3	R	336	NAD	O4D-C1D-N1N-C2N
3	R	336	NAD	O4D-C1D-N1N-C6N
3	R	336	NAD	C2D-C1D-N1N-C2N
3	R	336	NAD	C2D-C1D-N1N-C6N
3	O	336	NAD	O4B-C4B-C5B-O5B
3	R	336	NAD	PN-O3-PA-O1A
3	Q	336	NAD	O4B-C4B-C5B-O5B
3	P	336	NAD	PN-O3-PA-O2A
3	P	336	NAD	O4B-C4B-C5B-O5B
3	R	336	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	336	NAD	1	0
3	Q	336	NAD	1	0

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

Ligand NAD P 336

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD Q 336

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD O 336

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD R 336

Bond lengths

Bond angles

Torsions

Rings
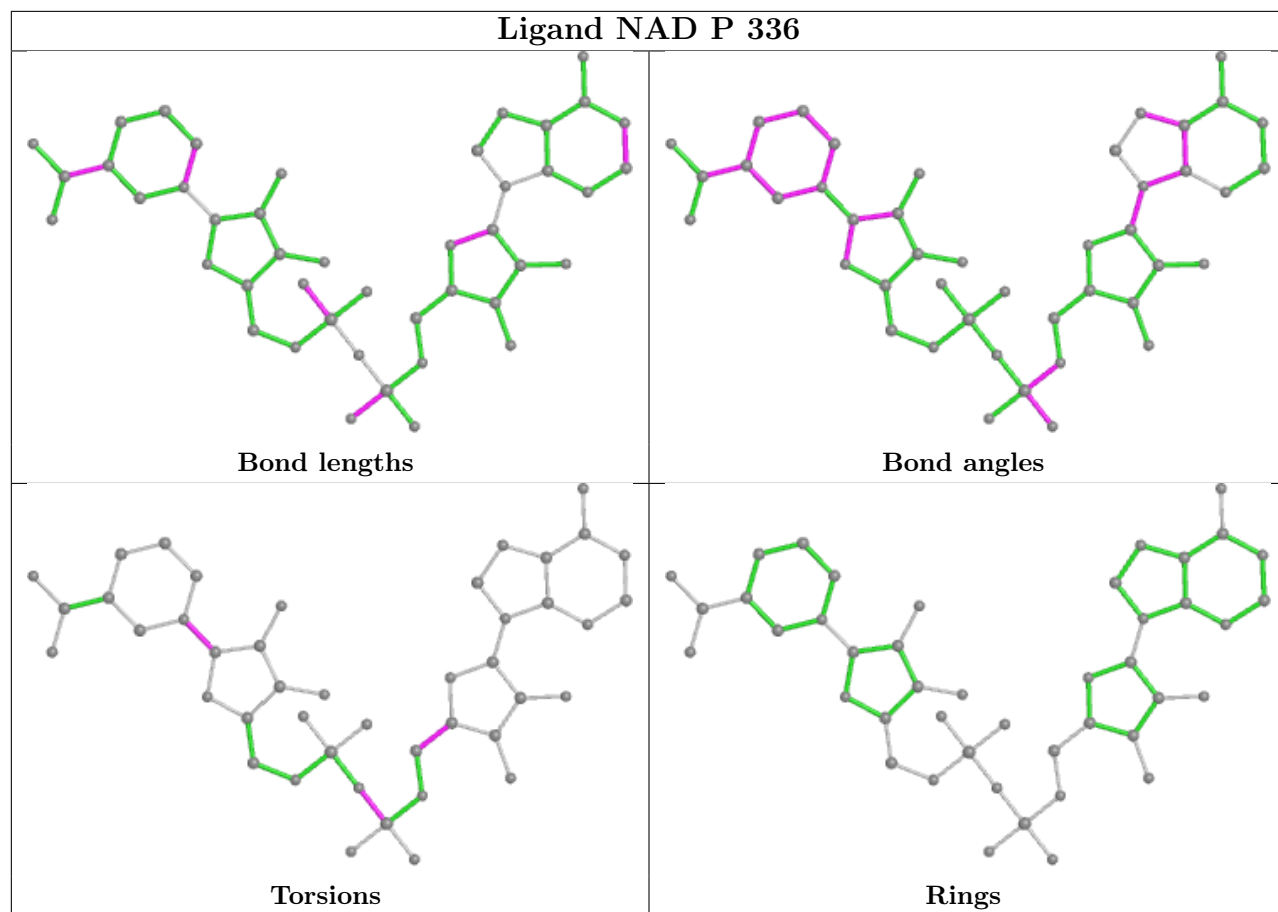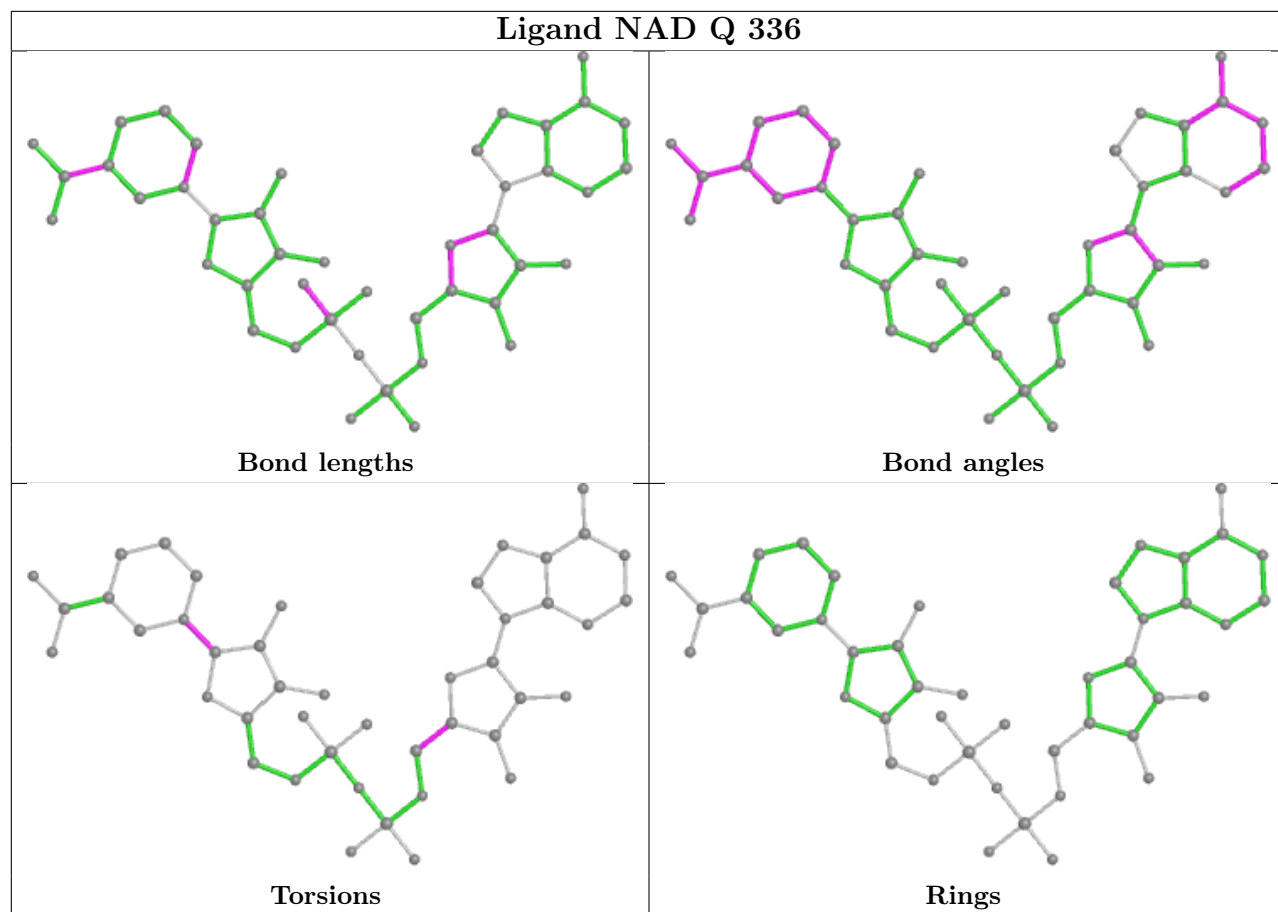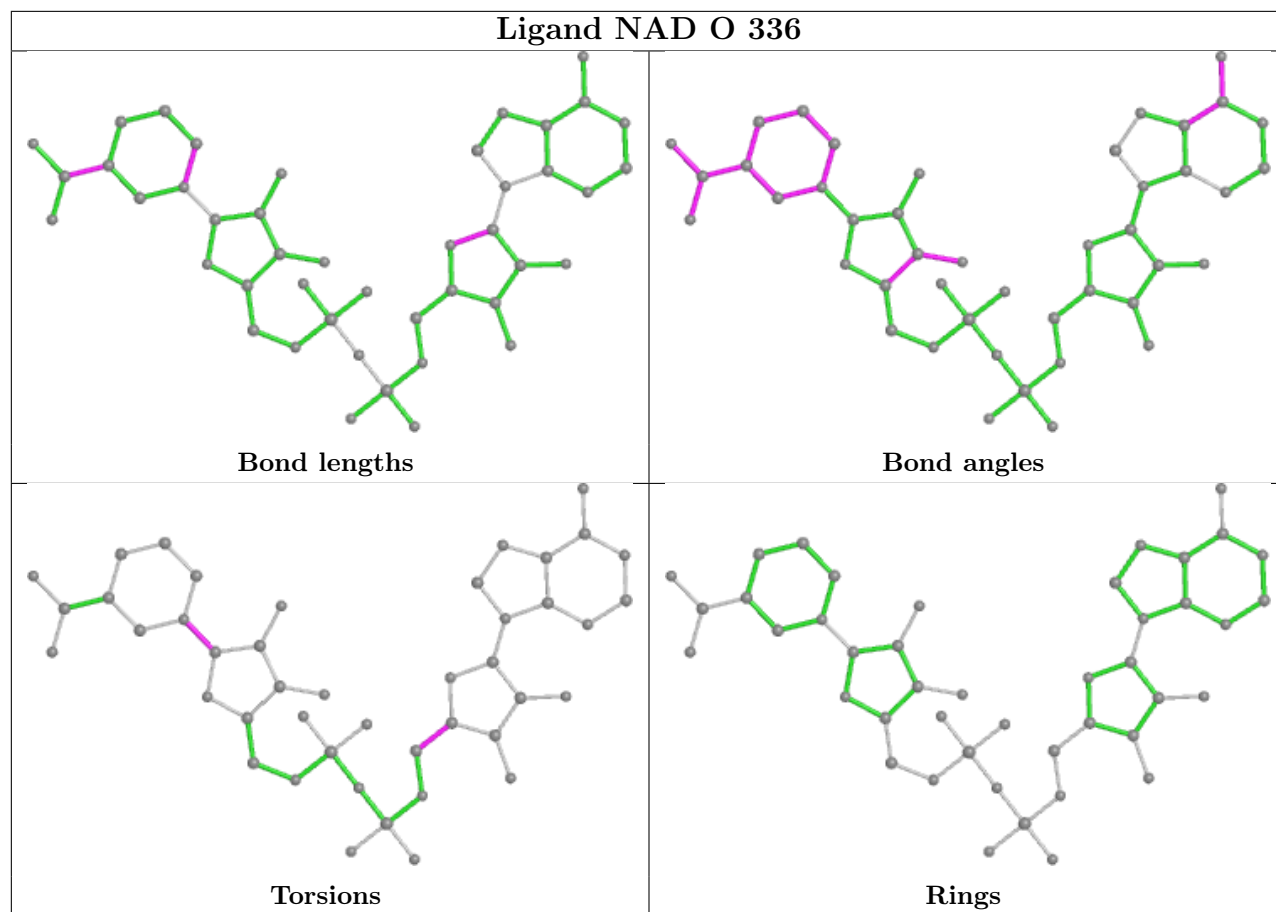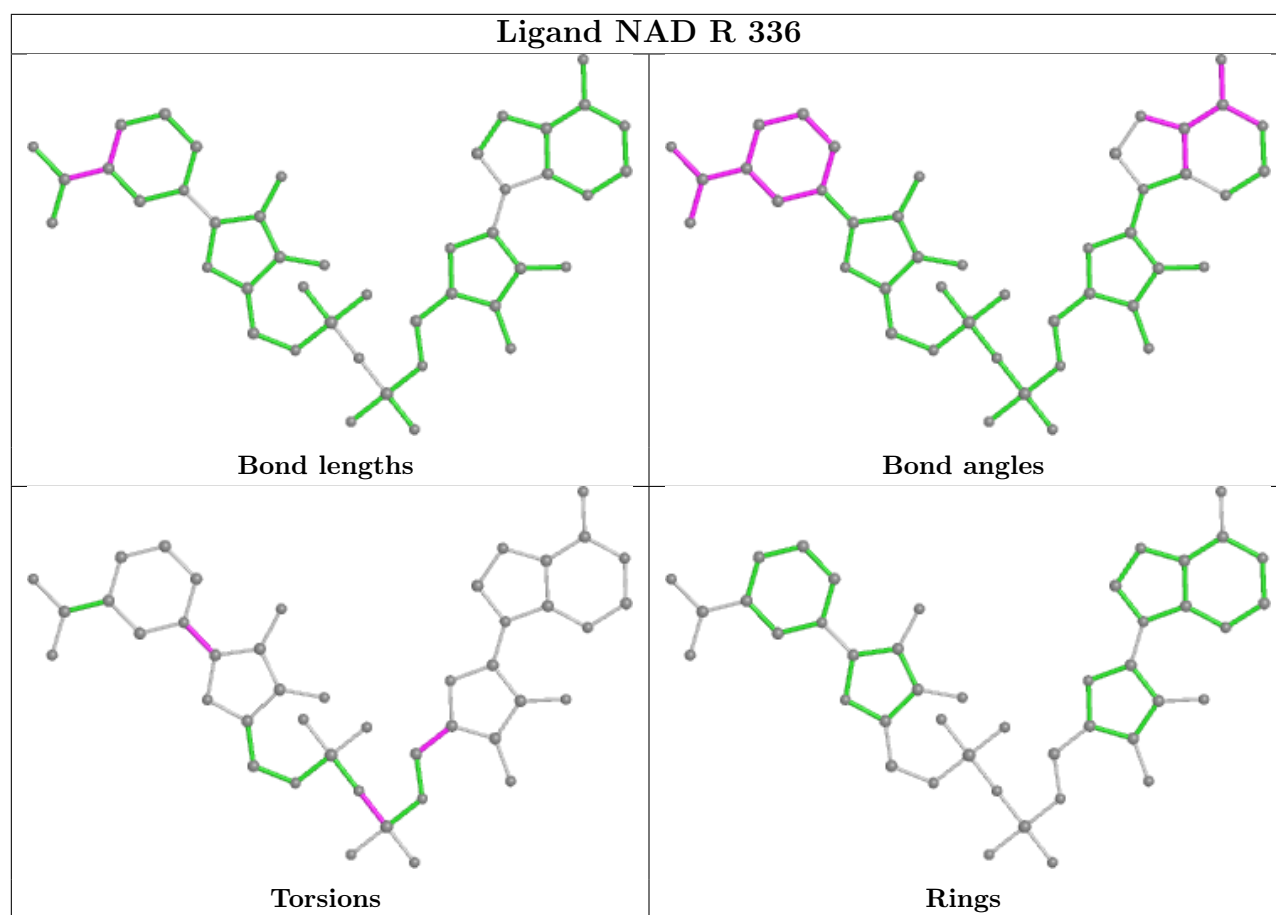
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	O	334/334 (100%)	-0.60	1 (0%)	94	92	4, 14, 37, 55	0
1	P	334/334 (100%)	-0.55	1 (0%)	94	92	3, 15, 37, 52	0
1	Q	334/334 (100%)	-0.52	2 (0%)	89	87	4, 16, 43, 59	0
1	R	334/334 (100%)	-0.60	2 (0%)	89	87	4, 14, 34, 60	0
All	All	1336/1336 (100%)	-0.57	6 (0%)	92	90	3, 15, 38, 60	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	61	GLY	2.8
1	P	333	LEU	2.2
1	R	62	ASN	2.1
1	O	62	ASN	2.0
1	Q	23	PRO	2.0
1	R	0	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

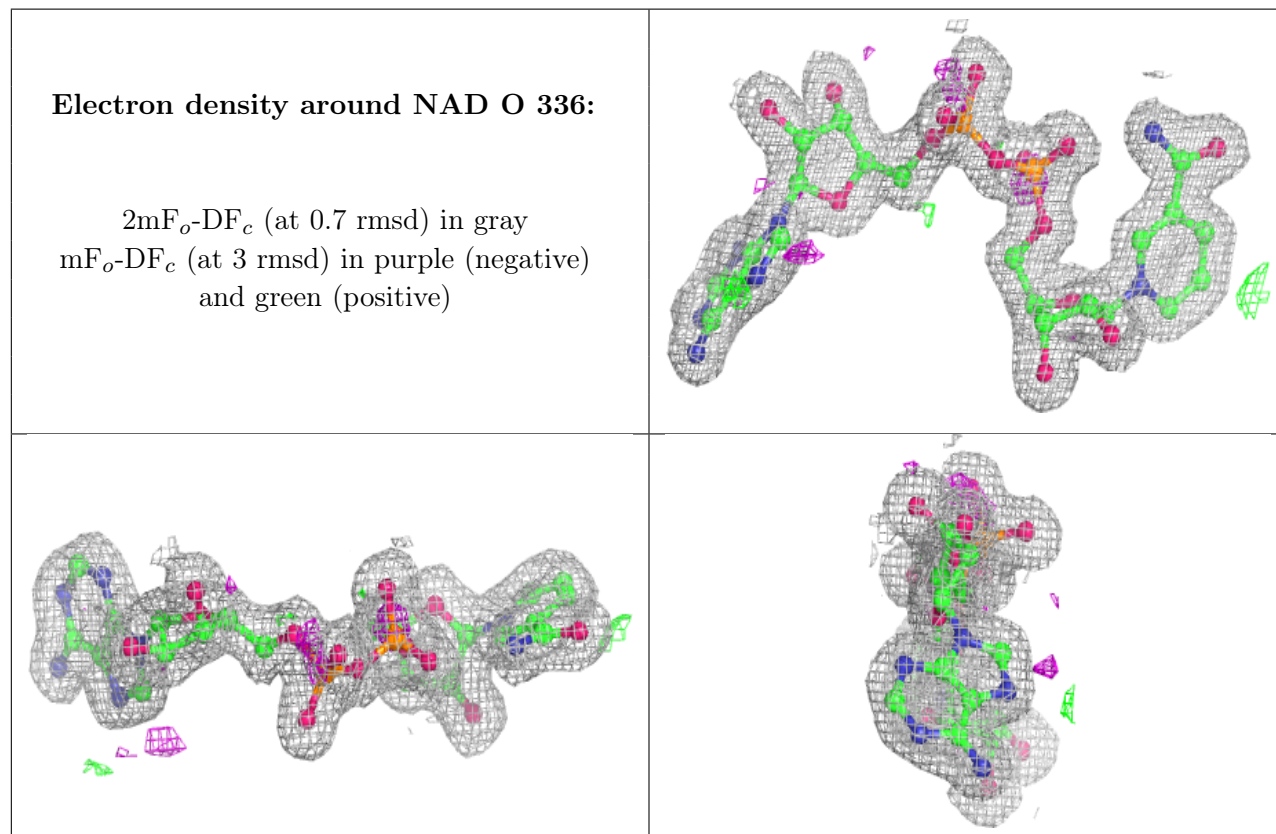## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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	SO4	R	339	5/5	0.90	0.18	26,27,32,38	0
2	SO4	P	339	5/5	0.96	0.19	30,31,34,36	0
2	SO4	Q	339	5/5	0.96	0.20	27,28,32,34	0
2	SO4	O	338	5/5	0.96	0.11	17,18,19,20	0
2	SO4	O	339	5/5	0.97	0.21	23,26,35,37	0
2	SO4	Q	338	5/5	0.97	0.09	20,24,26,28	0
2	SO4	P	338	5/5	0.98	0.14	33,35,39,40	0
3	NAD	O	336	44/44	0.98	0.05	5,9,16,19	0
3	NAD	P	336	44/44	0.98	0.06	4,10,12,17	0
3	NAD	Q	336	44/44	0.98	0.05	2,10,12,13	0
3	NAD	R	336	44/44	0.98	0.06	7,11,16,18	0
2	SO4	R	338	5/5	0.99	0.12	23,26,33,33	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.
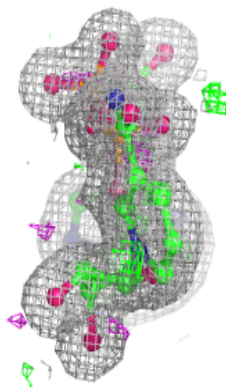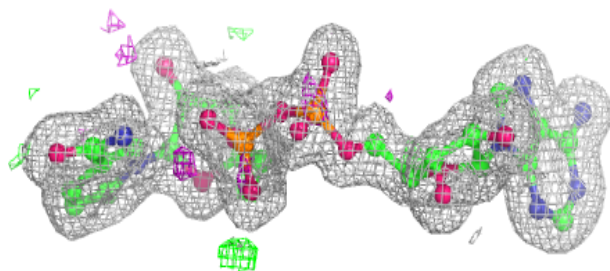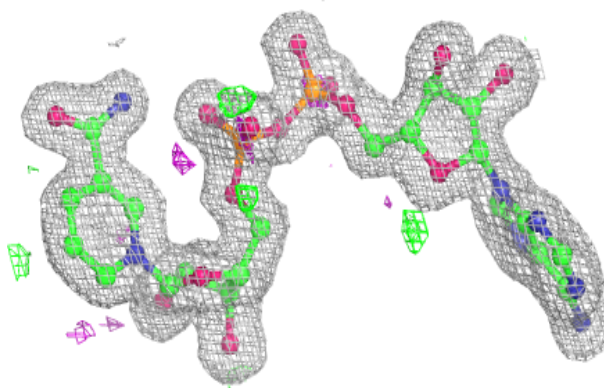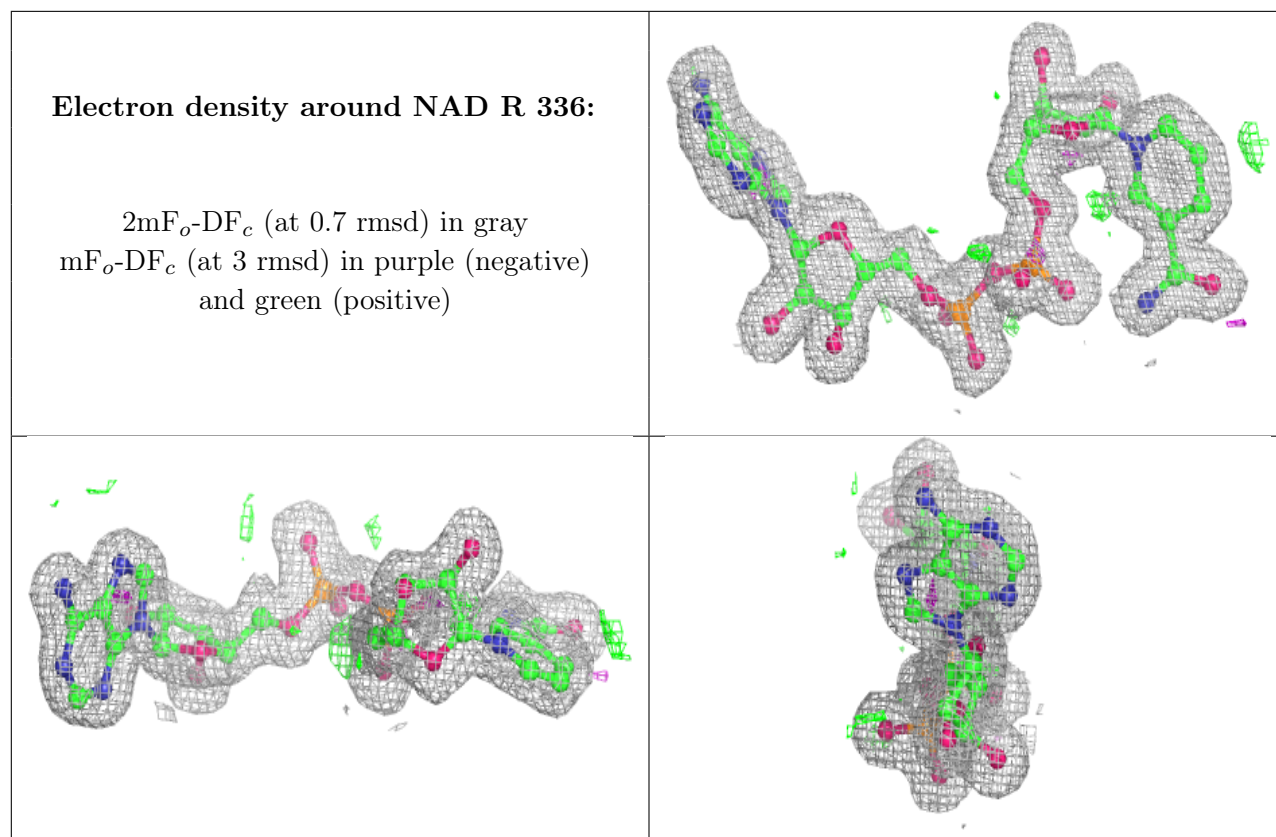

Electron density around NAD O 336:

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

Electron density around NAD P 336:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
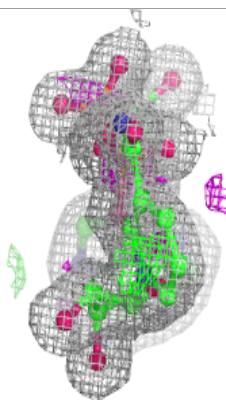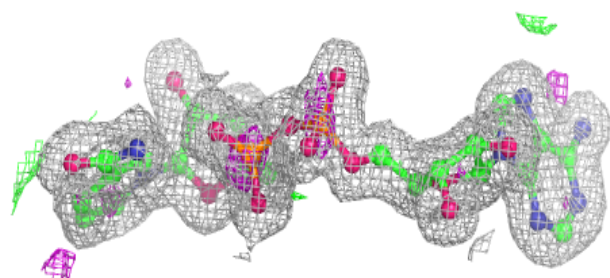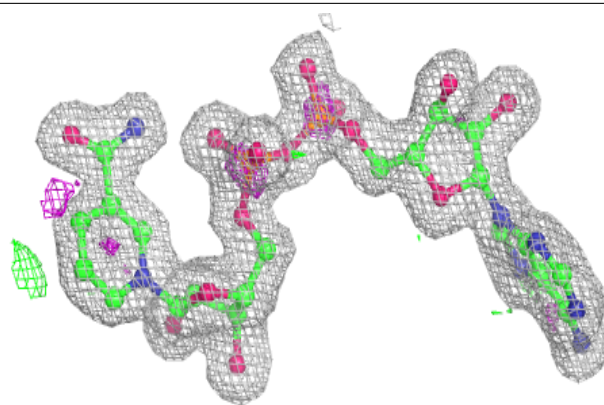
Electron density around NAD Q 336:

$2mF_o$-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 R 336:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.