



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:23 AM UTC

PDB ID : 1GD1 / pdb_00001gd1
Title : STRUCTURE OF HOLO-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

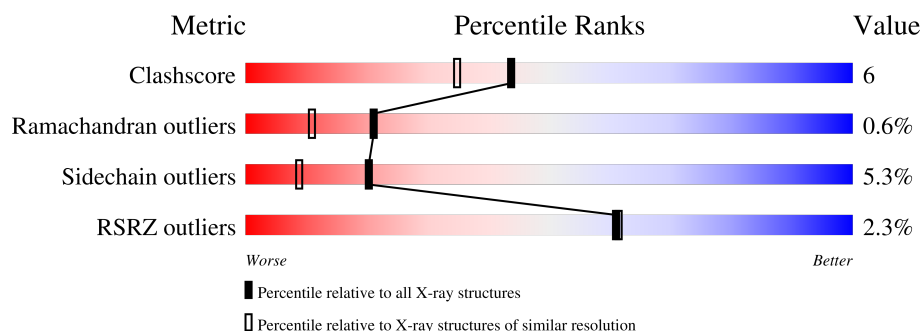
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	O	334	2% 69% 26% • •
1	P	334	% 69% 25% 5%
1	Q	334	4% 63% 32% • •
1	R	334	% 66% 29% • •

2 Entry composition [i](#)

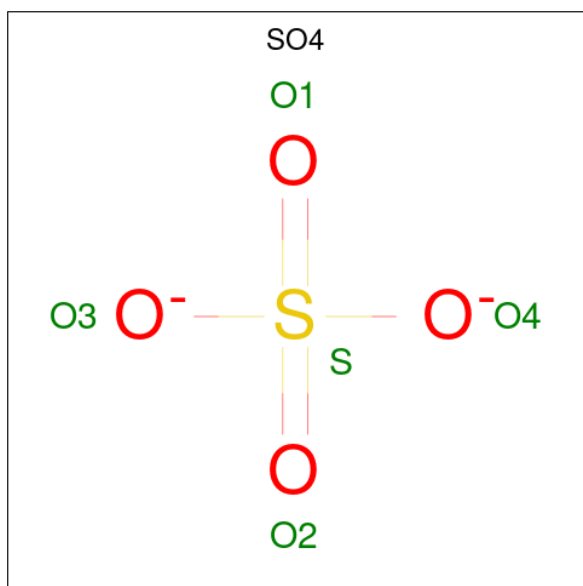
There are 4 unique types of molecules in this entry. The entry contains 10984 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DEHYDROGENASE.

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 (CCD ID: SO4) (formula: O₄S).



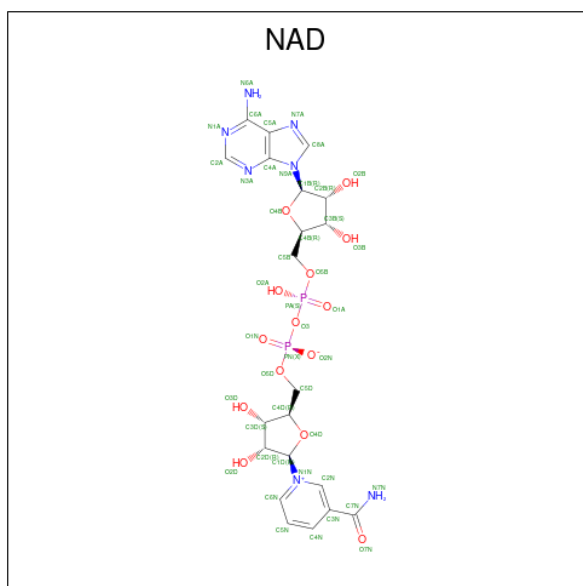
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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

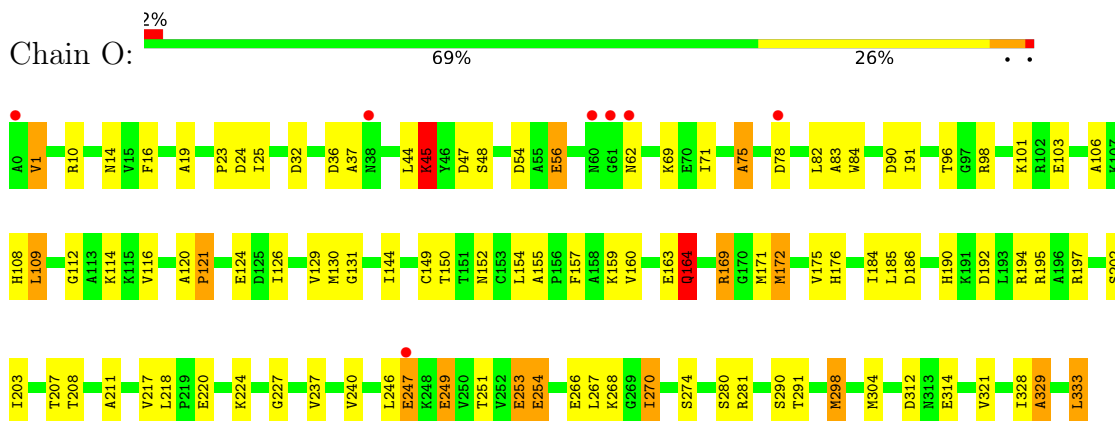
- Molecule 4 is water.

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

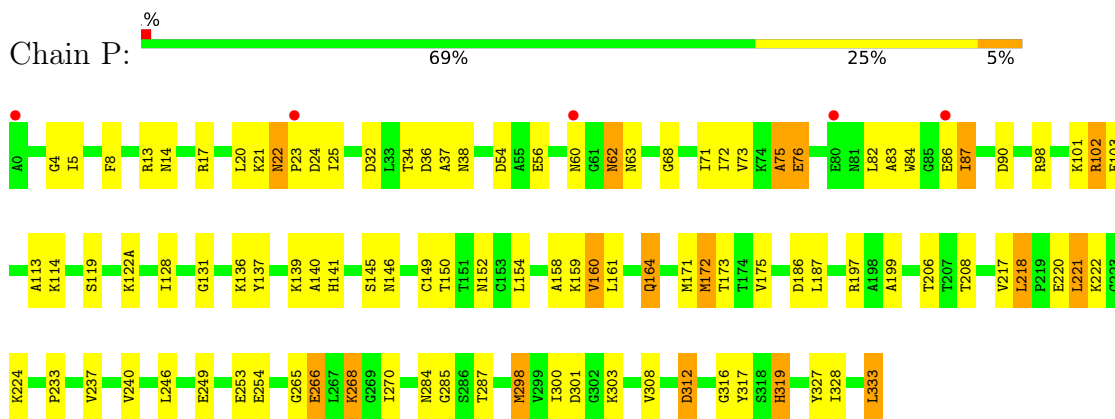
3 Residue-property plots

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.

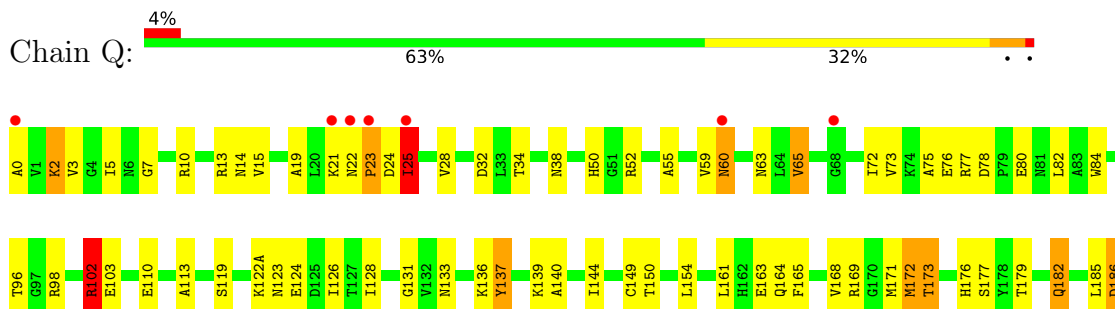
• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

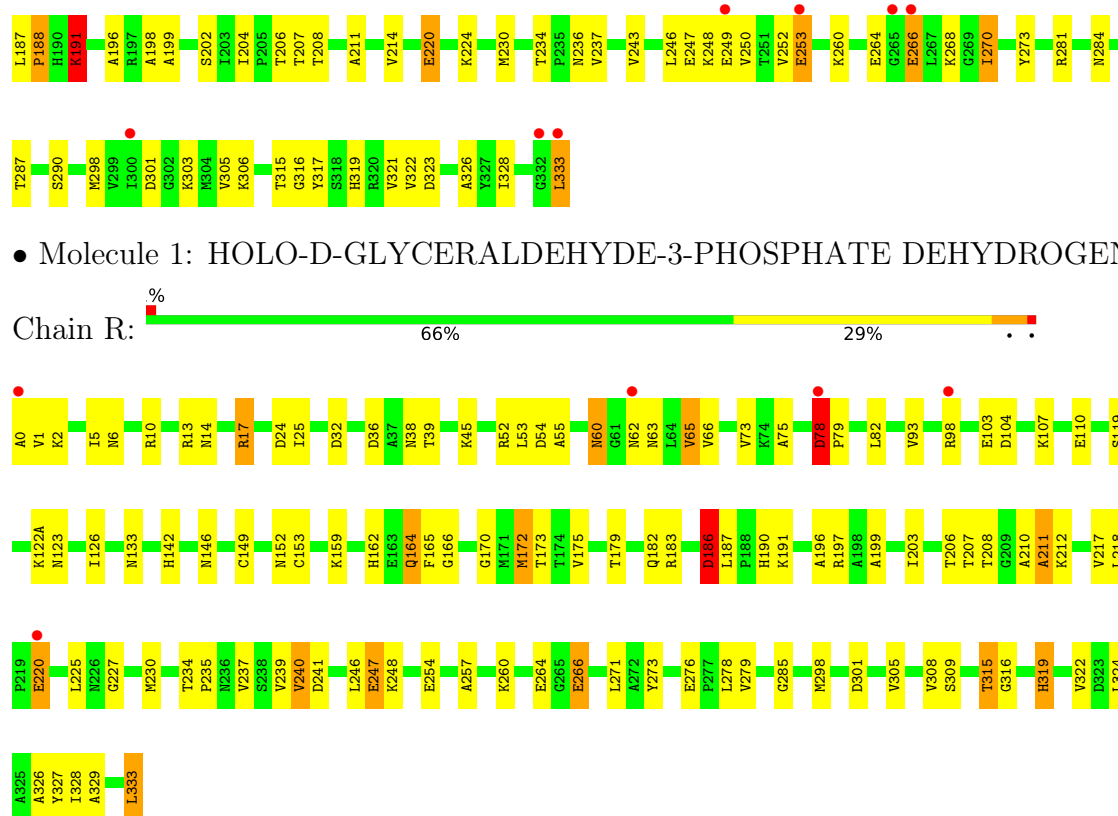


• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



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





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

Chain R: %

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 78.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 80.1 (78.05-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.37 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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 [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	1.40	6/2561 (0.2%)	2.12	85/3474 (2.4%)
1	P	1.44	8/2561 (0.3%)	2.10	77/3474 (2.2%)
1	Q	1.42	12/2561 (0.5%)	2.18	104/3474 (3.0%)
1	R	1.43	7/2561 (0.3%)	2.12	89/3474 (2.6%)
All	All	1.42	33/10244 (0.3%)	2.13	355/13896 (2.6%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	34	THR	CA-CB	6.62	1.62	1.53
1	P	187	LEU	N-CA	6.57	1.51	1.45
1	Q	273	TYR	N-CA	6.47	1.54	1.46
1	Q	187	LEU	N-CA	6.24	1.51	1.45
1	R	78	ASP	CG-OD2	6.23	1.37	1.25
1	P	4	GLY	N-CA	6.05	1.51	1.45
1	Q	72	ILE	CA-CB	5.95	1.60	1.54
1	Q	234	THR	CA-C	5.92	1.58	1.52
1	Q	204	ILE	CA-CB	5.89	1.59	1.54
1	R	315	THR	CA-CB	5.86	1.62	1.53
1	O	96	THR	CA-CB	5.79	1.62	1.53
1	Q	7	GLY	CA-C	5.59	1.59	1.51
1	R	186	ASP	CA-C	5.56	1.60	1.52
1	R	5	ILE	CA-CB	5.55	1.61	1.54
1	O	203	ILE	CA-C	5.53	1.59	1.52
1	R	239	VAL	C-O	5.49	1.29	1.24
1	Q	34	THR	CA-CB	5.45	1.61	1.53
1	R	119	SER	N-CA	5.44	1.53	1.46
1	P	312	ASP	CA-C	5.39	1.59	1.52
1	Q	315	THR	CA-CB	5.38	1.61	1.53
1	R	187	LEU	N-CA	5.36	1.50	1.45
1	Q	204	ILE	N-CA	5.30	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	56	GLU	N-CA	5.28	1.52	1.46
1	Q	207	THR	CA-CB	5.24	1.61	1.53
1	P	233	PRO	C-O	5.24	1.30	1.24
1	P	5	ILE	CA-CB	5.22	1.60	1.54
1	Q	5	ILE	CA-CB	5.14	1.60	1.54
1	P	101	LYS	N-CA	5.13	1.52	1.46
1	O	48	SER	C-N	-5.13	1.28	1.33
1	O	280	SER	C-O	5.12	1.29	1.24
1	O	150	THR	CA-CB	5.12	1.61	1.53
1	Q	96	THR	CA-CB	5.07	1.61	1.53
1	P	316	GLY	CA-C	5.01	1.57	1.52

All (355) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	266	GLU	CA-CB-CG	19.69	153.47	114.10
1	P	266	GLU	CB-CG-CD	14.03	136.44	112.60
1	O	217	VAL	CA-C-N	10.96	134.36	122.74
1	O	217	VAL	C-N-CA	10.96	134.36	122.74
1	R	266	GLU	CA-CB-CG	10.61	135.33	114.10
1	O	47	ASP	O-C-N	10.58	135.54	123.27
1	R	247	GLU	CB-CG-CD	9.66	129.03	112.60
1	P	152	ASN	OD1-CG-ND2	9.53	132.13	122.60
1	Q	182	GLN	OE1-CD-NE2	9.42	132.02	122.60
1	Q	110	GLU	CB-CG-CD	9.21	128.25	112.60
1	Q	266	GLU	CB-CG-CD	9.17	128.19	112.60
1	P	149	CYS	CA-C-N	8.90	132.20	120.28
1	P	149	CYS	C-N-CA	8.90	132.20	120.28
1	P	218	LEU	CA-C-O	8.85	131.49	121.22
1	Q	13	ARG	CD-NE-CZ	8.60	136.44	124.40
1	Q	78	ASP	CA-CB-CG	-8.59	104.02	112.60
1	R	98	ARG	NE-CZ-NH2	-8.55	111.50	119.20
1	Q	98	ARG	NE-CZ-NH2	-8.53	111.52	119.20
1	O	98	ARG	NE-CZ-NH2	-8.52	111.53	119.20
1	P	98	ARG	NE-CZ-NH2	-8.52	111.53	119.20
1	P	13	ARG	CD-NE-CZ	8.44	136.22	124.40
1	O	190	HIS	CA-C-O	-8.38	111.67	120.89
1	Q	13	ARG	NE-CZ-NH2	8.13	126.52	119.20
1	R	162	HIS	CA-CB-CG	-8.09	105.71	113.80
1	R	319	HIS	CA-CB-CG	-8.07	105.73	113.80
1	Q	60	ASN	OD1-CG-ND2	8.02	130.62	122.60
1	Q	60	ASN	CA-CB-CG	-7.92	104.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	164	GLN	N-CA-C	7.83	119.60	111.14
1	P	60	ASN	CA-CB-CG	-7.81	104.79	112.60
1	R	126	ILE	O-C-N	7.77	129.73	122.97
1	O	44	LEU	CA-C-N	7.76	130.99	120.44
1	O	44	LEU	C-N-CA	7.76	130.99	120.44
1	P	22	ASN	CA-C-O	7.69	125.01	119.32
1	Q	250	VAL	O-C-N	7.68	131.45	123.00
1	R	55	ALA	O-C-N	7.64	131.03	123.46
1	O	218	LEU	O-C-N	7.58	127.61	121.17
1	P	140	ALA	N-CA-C	7.57	123.66	113.97
1	Q	102	ARG	CB-CA-C	7.45	125.25	110.42
1	O	23	PRO	CA-C-N	7.44	134.16	121.14
1	O	23	PRO	C-N-CA	7.44	134.16	121.14
1	Q	154	LEU	N-CA-C	7.41	119.14	111.14
1	O	10	ARG	NE-CZ-NH1	7.36	128.86	121.50
1	P	173	THR	N-CA-CB	7.33	123.48	110.80
1	R	13	ARG	O-C-N	7.30	131.25	122.27
1	O	203	ILE	N-CA-CB	7.29	119.11	110.95
1	R	38	ASN	CA-CB-CG	-7.29	105.31	112.60
1	P	37	ALA	O-C-N	7.23	129.79	122.12
1	O	36	ASP	CA-CB-CG	-7.17	105.43	112.60
1	O	108	HIS	CA-C-N	7.17	130.19	120.44
1	O	108	HIS	C-N-CA	7.17	130.19	120.44
1	R	207	THR	CA-CB-OG1	-7.16	98.86	109.60
1	Q	281	ARG	N-CA-CB	7.14	121.22	110.22
1	R	13	ARG	CD-NE-CZ	7.13	134.38	124.40
1	P	37	ALA	CA-C-O	-7.11	113.01	120.55
1	P	317	TYR	CA-C-O	-7.01	113.46	120.82
1	O	124	GLU	CB-CG-CD	7.00	124.51	112.60
1	P	140	ALA	N-CA-CB	-7.00	100.94	110.67
1	O	195	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	P	146	ASN	OD1-CG-ND2	6.92	129.52	122.60
1	R	149	CYS	CB-CA-C	6.90	122.24	110.79
1	Q	177	SER	O-C-N	6.88	130.79	122.75
1	Q	113	ALA	CA-C-O	-6.88	113.89	121.87
1	R	98	ARG	NE-CZ-NH1	6.86	128.36	121.50
1	O	175	VAL	N-CA-C	-6.85	97.30	107.51
1	O	98	ARG	NE-CZ-NH1	6.84	128.34	121.50
1	O	176	HIS	N-CA-CB	-6.84	99.38	111.08
1	P	98	ARG	NE-CZ-NH1	6.84	128.34	121.50
1	O	274	SER	CA-C-O	6.82	127.89	120.32
1	Q	98	ARG	NE-CZ-NH1	6.80	128.31	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	177	SER	CA-C-O	-6.79	114.40	121.87
1	P	154	LEU	N-CA-C	6.77	118.74	111.36
1	O	71	ILE	CA-C-O	-6.69	113.39	120.48
1	R	301	ASP	CA-CB-CG	6.66	119.26	112.60
1	P	38	ASN	CA-CB-CG	-6.66	105.94	112.60
1	P	22	ASN	CB-CA-C	6.65	118.95	109.38
1	R	55	ALA	CA-C-O	-6.64	113.80	121.10
1	R	173	THR	N-CA-CB	6.63	122.27	110.80
1	Q	323	ASP	O-C-N	6.60	128.87	122.07
1	P	253	GLU	CB-CG-CD	6.60	123.81	112.60
1	O	109	LEU	O-C-N	6.59	129.21	122.09
1	Q	319	HIS	CA-CB-CG	-6.58	107.22	113.80
1	R	93	VAL	O-C-N	6.58	132.44	122.76
1	O	157	PHE	CA-CB-CG	6.57	120.37	113.80
1	R	203	ILE	N-CA-CB	6.54	118.46	111.00
1	P	102	ARG	NE-CZ-NH1	-6.54	114.96	121.50
1	Q	207	THR	O-C-N	6.54	130.24	122.79
1	R	13	ARG	CA-C-O	-6.54	112.45	119.97
1	R	10	ARG	NE-CZ-NH1	6.51	128.01	121.50
1	Q	77	ARG	CA-CB-CG	6.50	127.10	114.10
1	O	126	ILE	O-C-N	6.50	130.69	122.57
1	R	78	ASP	O-C-N	6.43	128.45	121.12
1	Q	326	ALA	CA-C-N	6.41	129.16	120.44
1	Q	326	ALA	C-N-CA	6.41	129.16	120.44
1	O	54	ASP	O-C-N	6.41	129.79	122.55
1	Q	173	THR	N-CA-CB	6.40	121.87	110.80
1	O	71	ILE	O-C-N	6.38	129.88	123.18
1	P	254	GLU	O-C-N	6.37	128.97	122.09
1	Q	315	THR	CA-C-O	-6.37	114.14	120.70
1	R	327	TYR	CA-C-N	6.37	129.19	120.46
1	R	327	TYR	C-N-CA	6.37	129.19	120.46
1	Q	214	VAL	CA-C-N	6.36	129.44	120.28
1	Q	214	VAL	C-N-CA	6.36	129.44	120.28
1	P	17	ARG	CD-NE-CZ	6.31	133.23	124.40
1	Q	50	HIS	CA-CB-CG	-6.30	107.50	113.80
1	O	154	LEU	N-CA-C	6.29	117.93	111.14
1	O	130	MET	CB-CA-C	6.29	119.27	109.84
1	P	73	VAL	CA-C-O	-6.28	113.81	120.53
1	R	146	ASN	CA-C-N	6.26	133.49	121.54
1	R	146	ASN	C-N-CA	6.26	133.49	121.54
1	Q	102	ARG	N-CA-CB	-6.24	99.94	110.49
1	R	36	ASP	CA-C-N	6.24	128.65	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	36	ASP	C-N-CA	6.24	128.65	120.28
1	R	199	ALA	O-C-N	6.24	128.73	122.12
1	R	254	GLU	O-C-N	6.24	128.49	122.07
1	P	161	LEU	O-C-N	6.23	128.73	122.12
1	P	8	PHE	CA-CB-CG	6.21	120.01	113.80
1	O	247	GLU	CB-CG-CD	6.20	123.14	112.60
1	Q	204	ILE	N-CA-CB	-6.18	104.99	111.36
1	Q	3	VAL	O-C-N	6.15	129.82	123.18
1	O	202	SER	CA-C-N	6.15	130.41	121.80
1	O	202	SER	C-N-CA	6.15	130.41	121.80
1	Q	161	LEU	CB-CG-CD2	6.15	129.15	110.70
1	Q	298	MET	N-CA-CB	-6.14	100.13	111.13
1	Q	163	GLU	CB-CG-CD	6.12	123.00	112.60
1	P	284	ASN	CA-C-O	-6.11	113.96	120.92
1	R	175	VAL	N-CA-C	-6.08	98.45	107.51
1	O	121	PRO	N-CA-C	-6.07	101.67	111.14
1	O	75	ALA	CA-C-N	6.07	130.72	122.84
1	O	75	ALA	C-N-CA	6.07	130.72	122.84
1	Q	136	LYS	CA-C-N	6.06	129.44	120.95
1	Q	136	LYS	C-N-CA	6.06	129.44	120.95
1	Q	50	HIS	CA-C-O	-6.06	112.47	119.56
1	R	14	ASN	CA-CB-CG	-6.04	106.56	112.60
1	O	207	THR	CA-CB-OG1	-6.03	100.55	109.60
1	Q	281	ARG	CA-C-O	-6.03	113.28	120.10
1	O	217	VAL	O-C-N	-6.03	116.17	122.20
1	R	183	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	R	60	ASN	CA-CB-CG	-6.01	106.59	112.60
1	Q	52	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	P	300	ILE	N-CA-CB	5.98	120.25	111.52
1	P	158	ALA	CA-C-N	5.97	129.08	120.79
1	P	158	ALA	C-N-CA	5.97	129.08	120.79
1	P	265	GLY	CA-C-N	5.96	128.59	120.54
1	P	265	GLY	C-N-CA	5.96	128.59	120.54
1	O	24	ASP	N-CA-C	5.96	120.28	112.89
1	P	54	ASP	CA-C-O	5.95	128.05	121.39
1	Q	176	HIS	N-CA-C	5.94	119.09	109.40
1	R	210	ALA	N-CA-C	5.92	119.32	111.75
1	P	75	ALA	CA-C-N	5.91	131.32	123.05
1	P	75	ALA	C-N-CA	5.91	131.32	123.05
1	Q	176	HIS	N-CA-CB	-5.91	100.55	110.83
1	Q	199	ALA	N-CA-C	5.91	117.72	111.28
1	R	285	GLY	CA-C-O	5.89	125.55	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	197	ARG	N-CA-C	5.88	119.18	110.48
1	O	116	VAL	O-C-N	5.88	129.55	123.20
1	Q	191	LYS	N-CA-CB	5.87	119.38	110.28
1	Q	23	PRO	CA-C-N	5.86	129.22	120.31
1	Q	23	PRO	C-N-CA	5.86	129.22	120.31
1	R	78	ASP	CB-CA-C	-5.86	103.67	110.17
1	Q	80	GLU	CA-C-N	5.84	132.61	122.56
1	Q	80	GLU	C-N-CA	5.84	132.61	122.56
1	O	1	VAL	CB-CA-C	5.83	118.72	111.15
1	R	211	ALA	O-C-N	5.81	129.78	122.23
1	Q	14	ASN	CB-CA-C	5.80	120.72	110.85
1	Q	55	ALA	CA-C-O	-5.79	114.73	121.10
1	R	182	GLN	OE1-CD-NE2	5.79	128.39	122.60
1	P	298	MET	N-CA-CB	-5.78	100.67	111.13
1	Q	96	THR	CA-C-N	5.77	132.50	122.05
1	Q	96	THR	C-N-CA	5.77	132.50	122.05
1	R	187	LEU	CA-C-O	5.77	126.35	120.64
1	O	290	SER	N-CA-CB	-5.76	101.14	110.71
1	Q	287	THR	CA-CB-OG1	-5.76	100.97	109.60
1	Q	301	ASP	CA-C-O	-5.75	113.53	120.32
1	P	141	HIS	CA-CB-CG	-5.73	108.07	113.80
1	R	230	MET	CA-C-O	-5.70	114.17	120.33
1	Q	322	VAL	CA-C-N	5.70	127.85	120.44
1	Q	322	VAL	C-N-CA	5.70	127.85	120.44
1	R	257	ALA	O-C-N	5.69	128.64	122.15
1	R	179	THR	CA-CB-OG1	-5.69	101.07	109.60
1	O	321	VAL	N-CA-CB	5.67	117.18	110.55
1	R	271	LEU	O-C-N	5.66	129.97	123.29
1	Q	198	ALA	CA-C-O	5.66	128.60	120.51
1	Q	179	THR	CA-CB-OG1	-5.65	101.13	109.60
1	P	175	VAL	O-C-N	5.64	129.76	122.77
1	Q	273	TYR	CA-C-N	-5.63	113.61	122.73
1	Q	273	TYR	C-N-CA	-5.63	113.61	122.73
1	O	45	LYS	CB-CA-C	-5.61	102.03	110.90
1	P	175	VAL	N-CA-C	-5.61	98.98	107.73
1	R	65	VAL	CA-C-O	-5.61	114.81	120.31
1	P	197	ARG	N-CA-C	5.59	118.75	110.48
1	O	270	ILE	O-C-N	5.59	126.95	121.98
1	R	197	ARG	N-CA-C	5.58	118.74	110.48
1	R	55	ALA	N-CA-C	-5.57	99.84	108.42
1	Q	204	ILE	N-CA-C	5.57	113.66	108.15
1	R	301	ASP	CA-C-N	5.55	132.30	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	301	ASP	C-N-CA	5.55	132.30	121.41
1	Q	317	TYR	CA-C-N	5.55	127.72	120.28
1	Q	317	TYR	C-N-CA	5.55	127.72	120.28
1	Q	133	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	P	316	GLY	O-C-N	5.54	127.50	122.18
1	Q	171	MET	O-C-N	5.54	130.03	123.27
1	O	240	VAL	O-C-N	5.53	128.79	122.93
1	O	14	ASN	CB-CA-C	5.53	120.25	110.85
1	Q	211	ALA	O-C-N	5.52	127.99	122.03
1	P	199	ALA	N-CA-C	5.50	117.36	111.36
1	P	36	ASP	CA-C-N	5.50	127.65	120.28
1	P	36	ASP	C-N-CA	5.50	127.65	120.28
1	Q	290	SER	N-CA-CB	-5.50	101.28	110.57
1	R	54	ASP	N-CA-CB	5.49	118.56	110.49
1	R	66	VAL	O-C-N	5.48	128.85	122.99
1	Q	140	ALA	N-CA-C	5.48	120.24	113.50
1	R	328	ILE	O-C-N	5.48	127.18	121.87
1	R	230	MET	CA-CB-CG	-5.47	103.16	114.10
1	R	142	HIS	CA-C-N	5.47	130.76	123.10
1	R	142	HIS	C-N-CA	5.47	130.76	123.10
1	R	6	ASN	CB-CA-C	5.46	119.52	110.78
1	R	211	ALA	N-CA-C	-5.46	104.98	111.69
1	R	316	GLY	N-CA-C	-5.45	106.18	112.50
1	R	62	ASN	N-CA-CB	-5.44	102.44	110.49
1	Q	52	ARG	CD-NE-CZ	5.43	132.01	124.40
1	O	91	ILE	CA-C-N	-5.43	116.03	123.14
1	O	91	ILE	C-N-CA	-5.43	116.03	123.14
1	O	254	GLU	N-CA-CB	5.42	118.19	110.16
1	Q	281	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	P	131	GLY	N-CA-C	-5.42	108.16	115.21
1	Q	187	LEU	O-C-N	-5.42	118.24	121.71
1	R	326	ALA	CA-C-N	5.41	127.47	120.44
1	R	326	ALA	C-N-CA	5.41	127.47	120.44
1	O	112	GLY	N-CA-C	5.40	122.20	114.64
1	Q	149	CYS	N-CA-C	-5.40	105.29	111.07
1	O	314	GLU	CA-C-N	5.39	127.78	120.44
1	O	314	GLU	C-N-CA	5.39	127.78	120.44
1	O	304	MET	CA-C-O	-5.38	114.60	120.36
1	Q	250	VAL	CA-C-O	-5.37	116.19	121.67
1	R	206	THR	CA-CB-OG1	-5.37	101.55	109.60
1	O	48	SER	CA-C-O	-5.36	114.04	120.10
1	P	14	ASN	CA-CB-CG	-5.36	107.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	221	LEU	CA-C-N	-5.36	113.34	120.90
1	P	221	LEU	C-N-CA	-5.36	113.34	120.90
1	P	4	GLY	N-CA-C	-5.36	102.08	111.46
1	R	190	HIS	CA-C-N	5.34	127.44	120.28
1	R	190	HIS	C-N-CA	5.34	127.44	120.28
1	O	164	GLN	N-CA-C	5.33	116.90	111.14
1	P	101	LYS	O-C-N	5.33	129.42	123.19
1	Q	270	ILE	CA-C-N	5.33	130.35	123.00
1	Q	270	ILE	C-N-CA	5.33	130.35	123.00
1	R	234	THR	CA-C-O	-5.32	114.45	120.46
1	Q	137	TYR	O-C-N	5.32	129.47	122.93
1	Q	315	THR	N-CA-C	5.29	116.85	111.14
1	O	129	VAL	N-CA-CB	5.29	118.56	111.90
1	O	333	LEU	N-CA-CB	-5.28	101.52	110.50
1	O	155	ALA	O-C-N	5.28	125.18	120.48
1	Q	15	VAL	O-C-N	-5.28	116.75	121.87
1	Q	266	GLU	CG-CD-OE1	5.28	130.53	118.40
1	O	25	ILE	CB-CA-C	5.27	118.56	110.55
1	O	253	GLU	CB-CG-CD	5.26	121.55	112.60
1	Q	149	CYS	CB-CA-C	5.26	119.14	110.88
1	P	287	THR	CA-CB-CG2	5.24	119.41	110.50
1	O	194	ARG	N-CA-C	-5.24	105.25	111.69
1	Q	281	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	P	63	ASN	O-C-N	5.23	130.24	122.97
1	O	130	MET	N-CA-CB	-5.23	101.38	109.48
1	Q	171	MET	N-CA-CB	5.23	120.46	111.00
1	P	303	LYS	N-CA-C	5.22	121.05	114.31
1	Q	52	ARG	CG-CD-NE	5.22	123.50	112.00
1	R	273	TYR	O-C-N	5.22	129.96	123.28
1	O	101	LYS	CA-CB-CG	5.21	124.52	114.10
1	O	249	GLU	CA-CB-CG	5.21	124.53	114.10
1	R	322	VAL	N-CA-CB	5.21	116.64	110.55
1	P	287	THR	CA-CB-OG1	-5.20	101.80	109.60
1	O	192	ASP	CA-C-O	-5.20	115.02	120.58
1	Q	188	PRO	CA-C-O	5.20	127.27	121.34
1	R	133	ASN	CB-CG-ND2	5.20	124.20	116.40
1	Q	202	SER	N-CA-C	5.20	116.70	108.96
1	P	13	ARG	NH1-CZ-NH2	-5.19	112.56	119.30
1	Q	303	LYS	CA-C-O	-5.18	113.38	119.24
1	O	152	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	R	264	GLU	CG-CD-OE2	-5.18	106.49	118.40
1	O	190	HIS	N-CA-C	-5.17	100.59	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	14	ASN	CB-CG-ND2	5.17	124.15	116.40
1	O	130	MET	CA-C-N	5.17	131.40	122.05
1	O	130	MET	C-N-CA	5.17	131.40	122.05
1	P	60	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	Q	199	ALA	CB-CA-C	-5.16	102.22	110.79
1	O	37	ALA	CA-C-N	5.16	127.14	120.44
1	O	37	ALA	C-N-CA	5.16	127.14	120.44
1	Q	253	GLU	CA-C-O	-5.16	115.08	120.55
1	O	149	CYS	CB-CA-C	5.16	119.35	110.79
1	P	327	TYR	CA-C-N	5.15	127.52	120.77
1	P	327	TYR	C-N-CA	5.15	127.52	120.77
1	R	279	VAL	CA-C-O	-5.15	116.41	121.67
1	R	305	VAL	O-C-N	5.15	128.51	123.00
1	P	217	VAL	CA-C-N	5.15	128.19	122.74
1	P	217	VAL	C-N-CA	5.15	128.19	122.74
1	O	314	GLU	CG-CD-OE2	-5.14	106.57	118.40
1	Q	25	ILE	CA-CB-CG2	5.14	119.23	110.50
1	R	5	ILE	O-C-N	5.14	128.65	123.20
1	P	285	GLY	CA-C-N	5.13	128.62	121.02
1	P	285	GLY	C-N-CA	5.13	128.62	121.02
1	P	317	TYR	CA-C-N	5.13	127.16	120.28
1	P	317	TYR	C-N-CA	5.13	127.16	120.28
1	Q	316	GLY	N-CA-C	-5.13	106.55	112.50
1	R	241	ASP	N-CA-CB	-5.13	101.79	110.46
1	P	145	SER	O-C-N	5.12	129.18	123.19
1	Q	284	ASN	CB-CA-C	5.12	117.53	110.16
1	R	52	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Q	65	VAL	CA-C-O	-5.12	115.07	120.39
1	Q	161	LEU	CB-CA-C	5.11	118.91	110.88
1	R	279	VAL	O-C-N	5.11	128.62	123.00
1	Q	76	GLU	CA-C-N	5.10	127.63	120.28
1	Q	76	GLU	C-N-CA	5.10	127.63	120.28
1	O	96	THR	CA-CB-OG1	-5.10	101.95	109.60
1	P	206	THR	CA-CB-OG1	-5.10	101.95	109.60
1	Q	206	THR	O-C-N	-5.10	117.77	123.48
1	O	312	ASP	O-C-N	5.10	129.40	122.57
1	P	20	LEU	CA-C-N	5.10	130.90	121.52
1	P	20	LEU	C-N-CA	5.10	130.90	121.52
1	P	68	GLY	CA-C-O	-5.08	114.17	119.20
1	Q	2	LYS	CB-CA-C	5.08	118.70	110.22
1	R	164	GLN	N-CA-C	5.08	117.94	111.69
1	O	169	ARG	CA-C-O	-5.08	115.80	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	76	GLU	CB-CA-C	-5.08	101.86	110.19
1	P	319	HIS	CA-CB-CG	-5.08	108.72	113.80
1	Q	321	VAL	N-CA-CB	5.07	116.49	110.55
1	R	309	SER	O-C-N	5.07	129.47	123.33
1	O	281	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	P	113	ALA	CA-C-O	-5.07	115.64	121.47
1	Q	124	GLU	CB-CG-CD	5.07	121.22	112.60
1	O	329	ALA	O-C-N	-5.06	116.86	122.07
1	Q	25	ILE	CB-CA-C	5.05	118.60	110.82
1	O	254	GLU	CA-C-O	-5.05	115.06	120.42
1	R	240	VAL	O-C-N	5.05	128.64	123.03
1	R	324	LEU	CA-C-N	5.05	127.01	120.44
1	R	324	LEU	C-N-CA	5.05	127.01	120.44
1	O	90	ASP	CA-CB-CG	-5.05	107.55	112.60
1	O	291	THR	N-CA-CB	5.05	118.51	110.84
1	R	153	CYS	CA-C-N	5.05	127.31	120.44
1	R	153	CYS	C-N-CA	5.05	127.31	120.44
1	P	160	VAL	CA-C-N	5.04	127.04	120.28
1	P	160	VAL	C-N-CA	5.04	127.04	120.28
1	O	321	VAL	N-CA-C	-5.04	105.58	110.42
1	R	152	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	Q	10	ARG	CA-C-O	5.04	126.11	120.82
1	R	17	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	R	217	VAL	CA-C-O	5.04	123.33	118.90
1	R	149	CYS	CA-C-N	5.04	127.03	120.28
1	R	149	CYS	C-N-CA	5.04	127.03	120.28
1	Q	236	ASN	CA-C-N	5.03	131.03	121.97
1	Q	236	ASN	C-N-CA	5.03	131.03	121.97
1	R	39	THR	CA-CB-OG1	-5.02	102.07	109.60
1	O	197	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	P	150	THR	CA-CB-OG1	-5.01	102.09	109.60
1	R	5	ILE	CA-C-N	-5.01	116.33	122.84
1	R	5	ILE	C-N-CA	-5.01	116.33	122.84
1	P	102	ARG	CG-CD-NE	-5.01	100.98	112.00

There are no chirality outliers.

There are no planarity outliers.

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	O	2525	0	2572	25	0
1	P	2525	0	2572	27	0
1	Q	2525	0	2572	44	0
1	R	2525	0	2572	34	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
4	P	162	0	0	3	0
4	Q	166	0	0	3	0
4	R	164	0	0	4	0
All	All	10984	0	10392	127	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 (127) 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:O:298:MET:HG2	1:P:171:MET:HE1	1.60	0.84
1:Q:220:GLU:H	1:Q:220:GLU:CD	1.89	0.79
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:172:MET:HE2	1:R:208:THR:HG21	1.81	0.62
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:O:171:MET:HE1	1:P:298:MET:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:220:GLU:H	1:R:220:GLU:CD	2.11	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:173:THR:HG21	1:Q:230:MET:HE3	1.87	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:224:LYS:NZ	4:O:471:HOH:O	2.41	0.53
1:O:251:THR:OG1	1:O:254:GLU:HG3	2.08	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:Q:150:THR:HG21	1:Q:172:MET:HE1	1.91	0.51
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:P:224:LYS:NZ	4:P:464:HOH:O	2.28	0.50
1:O:144:ILE:HD13	1:O:328:ILE:CD1	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:2:LYS:NZ	4:R:468:HOH:O	2.45	0.48
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:R:186:ASP:HA	1:R:196:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:185:LEU:O	1:Q:186:ASP:C	2.59	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:P:221:LEU:O	1:P:222:LYS:C	2.58	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
1:P:139:LYS:HD2	1:P:139:LYS:HA	1.80	0.43
1:Q:220:GLU:CD	1:Q:220:GLU:N	2.68	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:R:220:GLU:CD	1:R:220:GLU:N	2.74	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:Q:253:GLU:H	1:Q:253:GLU:CD	2.28	0.42
1:R:276:GLU:HB2	1:R:278:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:298:MET:HE3	1:R:298:MET:HB2	1.91	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:Q:306:LYS:NZ	4:Q:501:HOH:O	2.53	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:P:298:MET:HE3	1:P:298:MET:HB2	1.76	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:Q:172:MET:HE2	1:Q:208:THR:HG21	2.03	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:P:312:ASP:OD2	1:P:312:ASP:C	2.64	0.40
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
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 [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	O	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	21	11
1	P	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	21	11
1	Q	332/334 (99%)	316 (95%)	14 (4%)	2 (1%)	21	11
1	R	332/334 (99%)	318 (96%)	12 (4%)	2 (1%)	21	11
All	All	1328/1336 (99%)	1264 (95%)	56 (4%)	8 (1%)	21	11

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%)	256 (94%)	16 (6%)	18	7
1	P	272/272 (100%)	254 (93%)	18 (7%)	15	5
1	Q	272/272 (100%)	257 (94%)	15 (6%)	19	8
1	R	272/272 (100%)	263 (97%)	9 (3%)	33	21
All	All	1088/1088 (100%)	1030 (95%)	58 (5%)	20	9

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	45	LYS
1	O	56	GLU
1	O	62	ASN
1	O	69	LYS
1	O	78	ASP
1	O	103	GLU
1	O	164	GLN
1	O	172	MET
1	O	220	GLU
1	O	246	LEU
1	O	247	GLU
1	O	249	GLU
1	O	253	GLU
1	O	268	LYS
1	O	298	MET
1	O	333	LEU
1	P	23	PRO
1	P	25	ILE
1	P	56	GLU
1	P	62	ASN
1	P	71	ILE
1	P	87	ILE
1	P	103	GLU
1	P	122(A)	LYS
1	P	136	LYS
1	P	164	GLN
1	P	172	MET
1	P	220	GLU
1	P	246	LEU
1	P	249	GLU
1	P	266	GLU
1	P	268	LYS
1	P	270	ILE
1	P	333	LEU
1	Q	21	LYS
1	Q	25	ILE
1	Q	102	ARG
1	Q	103	GLU
1	Q	122(A)	LYS
1	Q	126	ILE
1	Q	172	MET
1	Q	191	LYS
1	Q	220	GLU

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Mol	Chain	Res	Type
1	Q	246	LEU
1	Q	249	GLU
1	Q	252	VAL
1	Q	266	GLU
1	Q	268	LYS
1	Q	333	LEU
1	R	78	ASP
1	R	172	MET
1	R	212	LYS
1	R	220	GLU
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	62	ASN
1	O	81	ASN
1	O	146	ASN
1	O	256	ASN
1	P	62	ASN
1	P	63	ASN
1	P	146	ASN
1	P	256	ASN
1	Q	38	ASN
1	Q	63	ASN
1	Q	81	ASN
1	Q	146	ASN
1	Q	256	ASN
1	Q	319	HIS
1	R	14	ASN
1	R	63	ASN
1	R	123	ASN
1	R	146	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 oligosaccharides 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	O	338	-	4,4,4	0.70	0	6,6,6	0.61	0
3	NAD	Q	336	-	46,48,48	1.48	6 (13%)	64,73,73	1.78	13 (20%)
2	SO4	R	338	-	4,4,4	0.65	0	6,6,6	0.55	0
2	SO4	R	339	-	4,4,4	0.90	0	6,6,6	0.50	0
3	NAD	P	336	-	46,48,48	1.57	7 (15%)	64,73,73	1.58	11 (17%)
2	SO4	P	338	-	4,4,4	0.60	0	6,6,6	0.67	0
2	SO4	O	339	-	4,4,4	1.22	0	6,6,6	0.74	0
2	SO4	Q	339	-	4,4,4	1.14	0	6,6,6	0.44	0
2	SO4	Q	338	-	4,4,4	0.82	0	6,6,6	1.19	1 (16%)
3	NAD	R	336	-	46,48,48	1.38	4 (8%)	64,73,73	1.93	12 (18%)
2	SO4	P	339	-	4,4,4	0.94	0	6,6,6	0.48	0
3	NAD	O	336	-	46,48,48	1.36	4 (8%)	64,73,73	1.89	12 (18%)

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	R	336	-	-	5/30/62/62	0/5/5/5
3	NAD	Q	336	-	-	6/30/62/62	0/5/5/5
3	NAD	O	336	-	-	5/30/62/62	0/5/5/5
3	NAD	P	336	-	-	7/30/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	336	NAD	PA-O3	-5.52	1.53	1.59
3	Q	336	NAD	C3N-C7N	5.35	1.58	1.50
3	R	336	NAD	PN-O3	-5.08	1.54	1.59
3	P	336	NAD	C3N-C7N	4.73	1.57	1.50
3	R	336	NAD	C3N-C7N	4.66	1.57	1.50
3	O	336	NAD	C3N-C7N	4.06	1.56	1.50
3	O	336	NAD	PN-O3	-4.04	1.55	1.59
3	O	336	NAD	PA-O3	-3.51	1.55	1.59
3	Q	336	NAD	PN-O3	-3.04	1.56	1.59
3	O	336	NAD	C6N-N1N	2.99	1.42	1.35
3	Q	336	NAD	PN-O2N	-2.91	1.41	1.55
3	Q	336	NAD	C8A-N7A	2.76	1.37	1.31
3	Q	336	NAD	O4B-C4B	2.63	1.50	1.45
3	P	336	NAD	PN-O2N	-2.55	1.43	1.55
3	Q	336	NAD	C6N-N1N	2.55	1.41	1.35
3	R	336	NAD	C4N-C3N	2.44	1.43	1.39
3	P	336	NAD	PN-O3	-2.42	1.56	1.59
3	P	336	NAD	C6N-N1N	2.39	1.40	1.35
3	P	336	NAD	C2A-N1A	2.17	1.37	1.33
3	R	336	NAD	C2N-N1N	2.06	1.37	1.35
3	P	336	NAD	PA-O1A	-2.04	1.43	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	336	NAD	C5N-C4N-C3N	-6.86	113.62	120.36
3	O	336	NAD	C5N-C6N-N1N	-5.90	112.34	120.38
3	R	336	NAD	O7N-C7N-C3N	-5.69	112.63	119.60
3	O	336	NAD	C6N-N1N-C2N	5.21	126.31	121.88
3	Q	336	NAD	C2N-C3N-C4N	4.59	123.59	118.26
3	Q	336	NAD	C4N-C3N-C7N	-4.59	108.57	121.06
3	O	336	NAD	C5N-C4N-C3N	-4.50	115.94	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	336	NAD	C6N-C5N-C4N	4.46	125.88	119.45
3	R	336	NAD	C4N-C3N-C7N	-4.46	108.92	121.06
3	O	336	NAD	C6N-C5N-C4N	4.42	125.82	119.45
3	Q	336	NAD	C5N-C6N-N1N	-4.29	114.53	120.38
3	P	336	NAD	C5N-C4N-C3N	-4.22	116.22	120.36
3	R	336	NAD	C2N-C3N-C4N	4.11	123.04	118.26
3	Q	336	NAD	C5N-C4N-C3N	-4.10	116.34	120.36
3	O	336	NAD	C4N-C3N-C7N	-4.05	110.04	121.06
3	P	336	NAD	C4N-C3N-C7N	-3.73	110.89	121.06
3	Q	336	NAD	O4B-C1B-N9A	-3.73	100.93	108.09
3	R	336	NAD	C5N-C6N-N1N	-3.69	115.35	120.38
3	P	336	NAD	C5N-C6N-N1N	-3.58	115.50	120.38
3	O	336	NAD	C3N-C7N-N7N	3.53	122.09	117.74
3	Q	336	NAD	C6N-N1N-C2N	3.45	124.81	121.88
3	R	336	NAD	O4B-C1B-N9A	-3.38	101.60	108.09
3	Q	336	NAD	C2A-N1A-C6A	3.32	124.19	118.73
3	P	336	NAD	C6N-N1N-C2N	3.32	124.70	121.88
3	P	336	NAD	C2N-C3N-C4N	3.30	122.09	118.26
3	Q	336	NAD	C6N-C5N-C4N	3.13	123.96	119.45
3	Q	336	NAD	O7N-C7N-C3N	-3.11	115.80	119.60
3	O	336	NAD	C2N-C3N-C4N	3.10	121.87	118.26
3	O	336	NAD	C2N-C3N-C7N	2.99	128.09	119.46
3	P	336	NAD	C6N-C5N-C4N	2.93	123.67	119.45
3	R	336	NAD	C2N-C3N-C7N	2.92	127.89	119.46
3	Q	336	NAD	C2N-C3N-C7N	2.90	127.84	119.46
3	R	336	NAD	N6A-C6A-N1A	2.85	124.73	118.38
3	O	336	NAD	O4B-C1B-N9A	-2.77	102.76	108.09
3	R	336	NAD	O7N-C7N-N7N	2.76	126.61	122.62
3	O	336	NAD	O3D-C3D-C4D	-2.67	103.41	111.08
3	Q	336	NAD	O7N-C7N-N7N	2.65	126.44	122.62
3	Q	336	NAD	N3A-C2A-N1A	-2.64	124.59	128.58
3	O	336	NAD	O2A-PA-O3	2.63	114.37	107.27
3	P	336	NAD	C2N-C3N-C7N	2.60	126.97	119.46
3	P	336	NAD	O4B-C1B-N9A	-2.48	103.33	108.09
3	R	336	NAD	C3N-C7N-N7N	2.45	120.76	117.74
3	O	336	NAD	O7N-C7N-C3N	-2.42	116.64	119.60
3	P	336	NAD	O2A-PA-O5B	-2.30	97.16	107.57
3	P	336	NAD	C4D-O4D-C1D	-2.28	107.84	109.92
2	Q	338	SO4	O4-S-O1	2.25	121.34	109.56
3	P	336	NAD	C4B-O4B-C1B	-2.10	104.84	109.47
3	Q	336	NAD	C6N-N1N-C1D	-2.09	115.63	119.73
3	R	336	NAD	C6N-N1N-C2N	2.03	123.60	121.88

There are no chirality outliers.

All (23) 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	R	336	NAD	PN-O3-PA-O1A
3	O	336	NAD	O4B-C4B-C5B-O5B
3	P	336	NAD	PN-O3-PA-O2A
3	Q	336	NAD	O4B-C4B-C5B-O5B
3	P	336	NAD	C2B-C1B-N9A-C8A
3	Q	336	NAD	C2B-C1B-N9A-C8A
3	P	336	NAD	PN-O3-PA-O1A

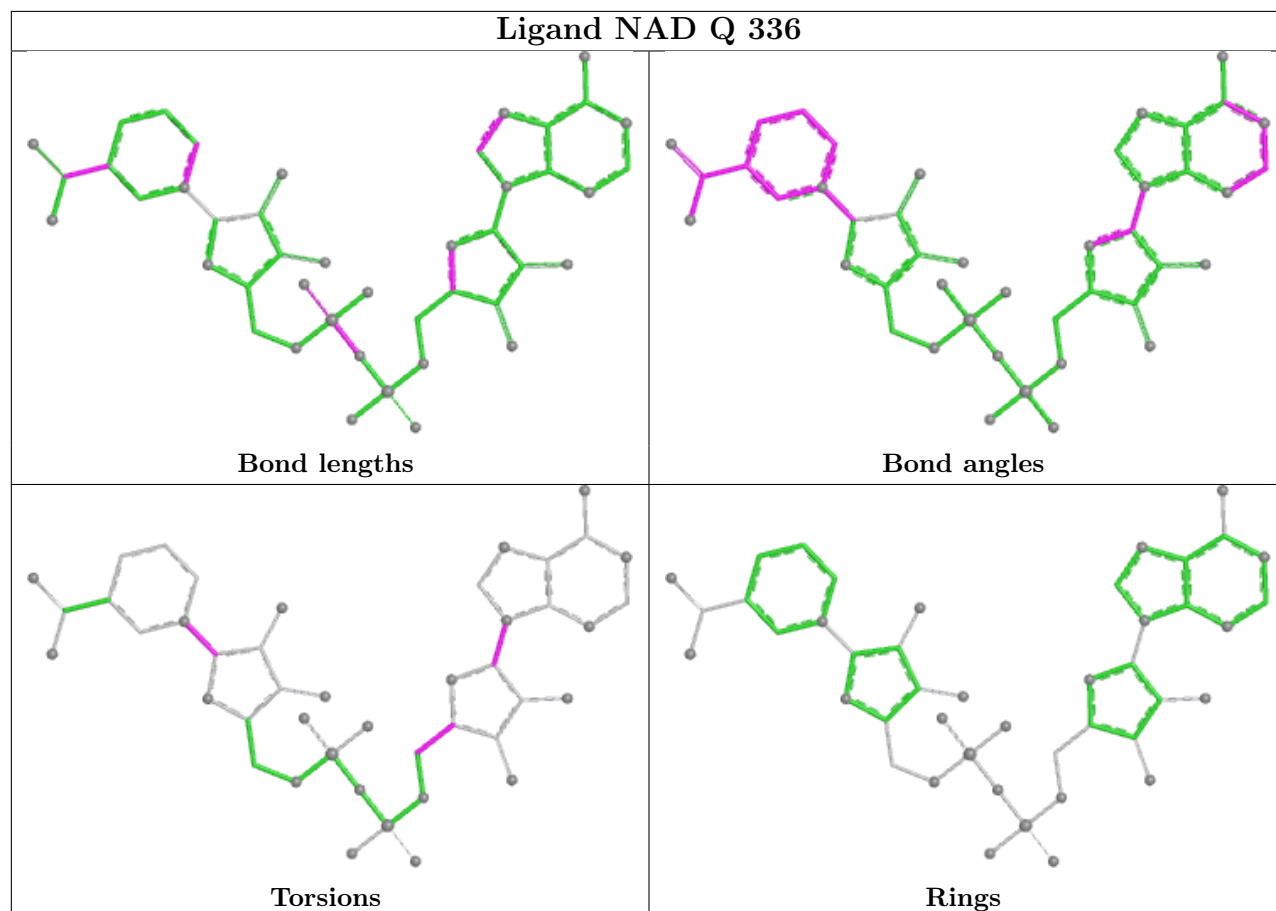
There are no ring outliers.

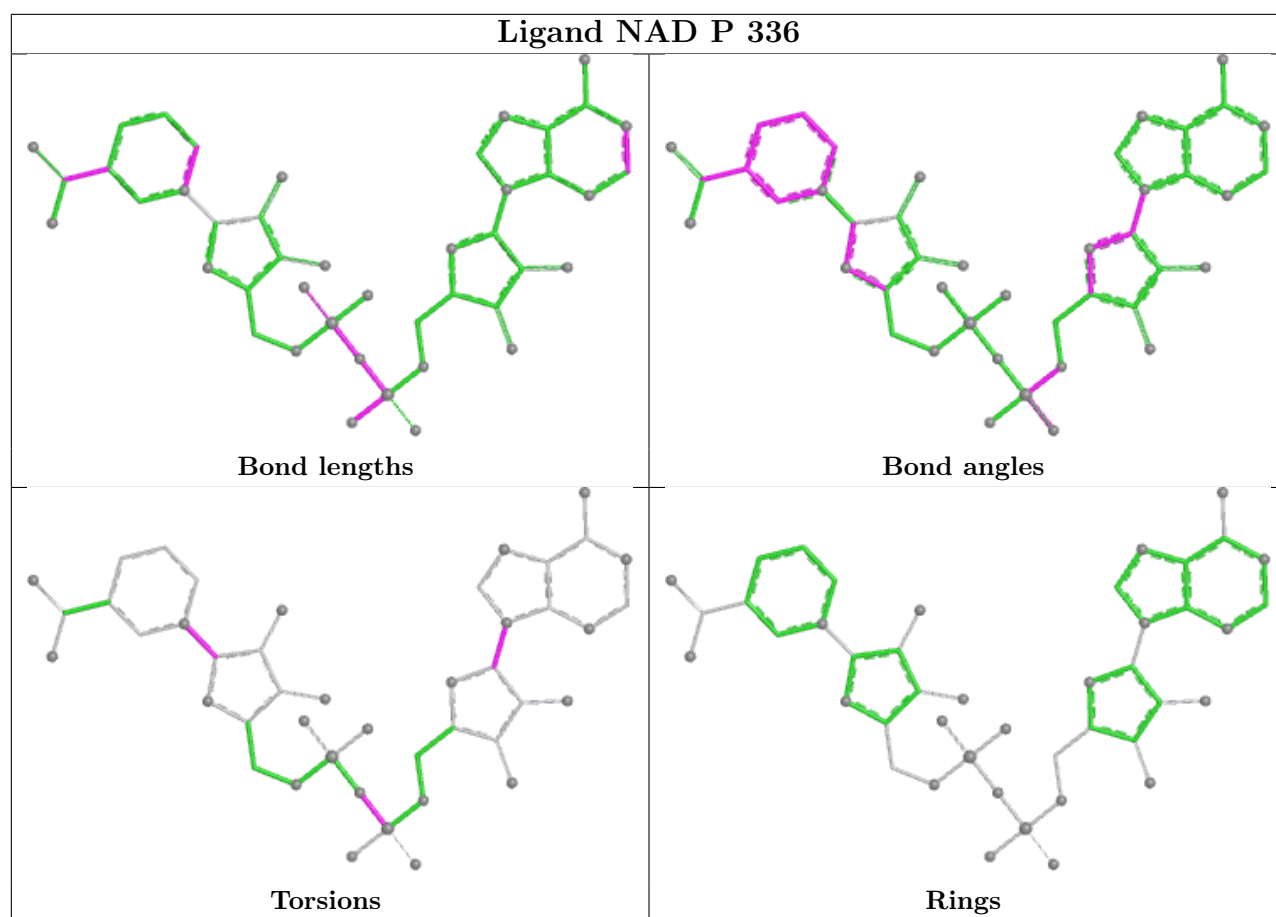
2 monomers are involved in 2 short contacts:

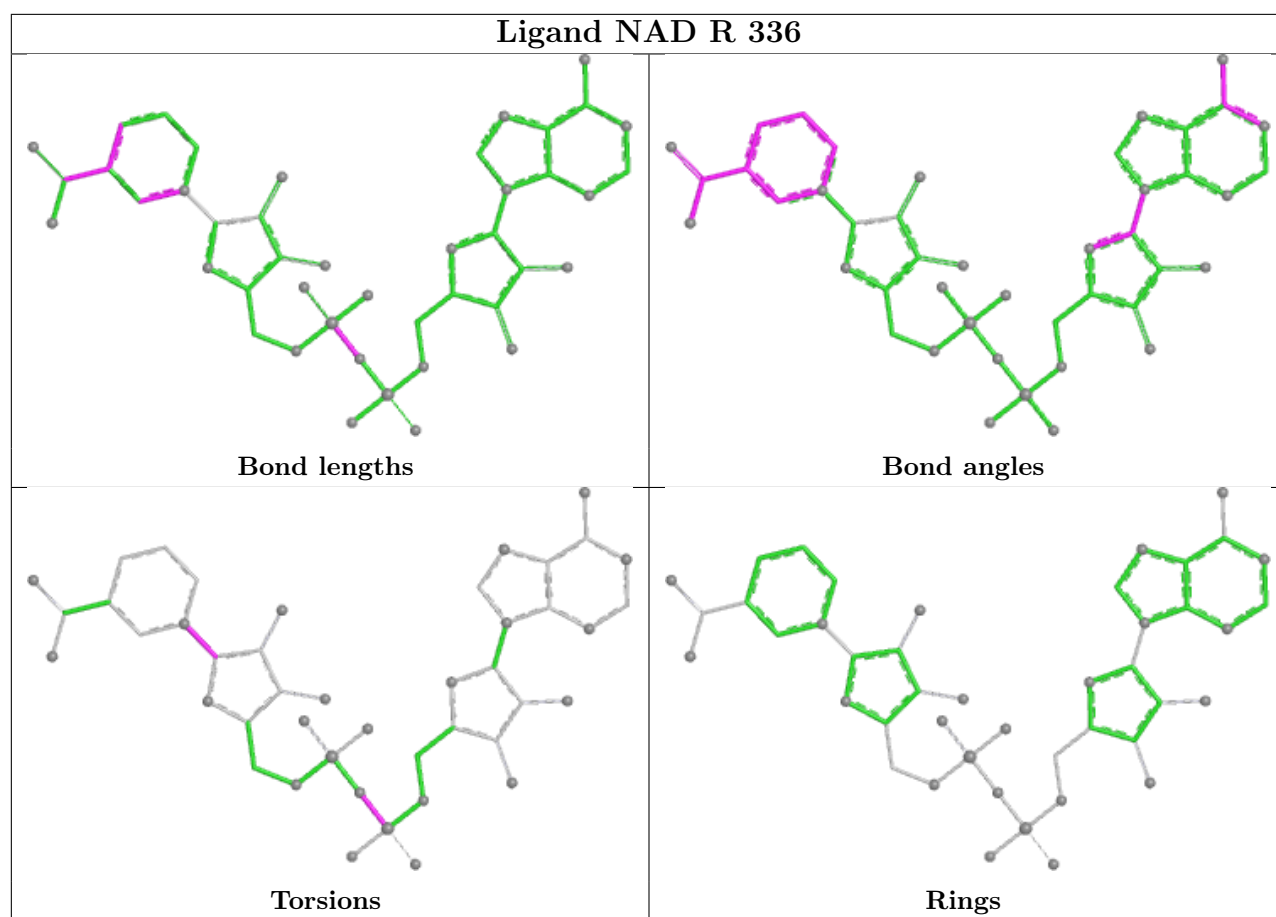
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	336	NAD	1	0
3	P	336	NAD	1	0

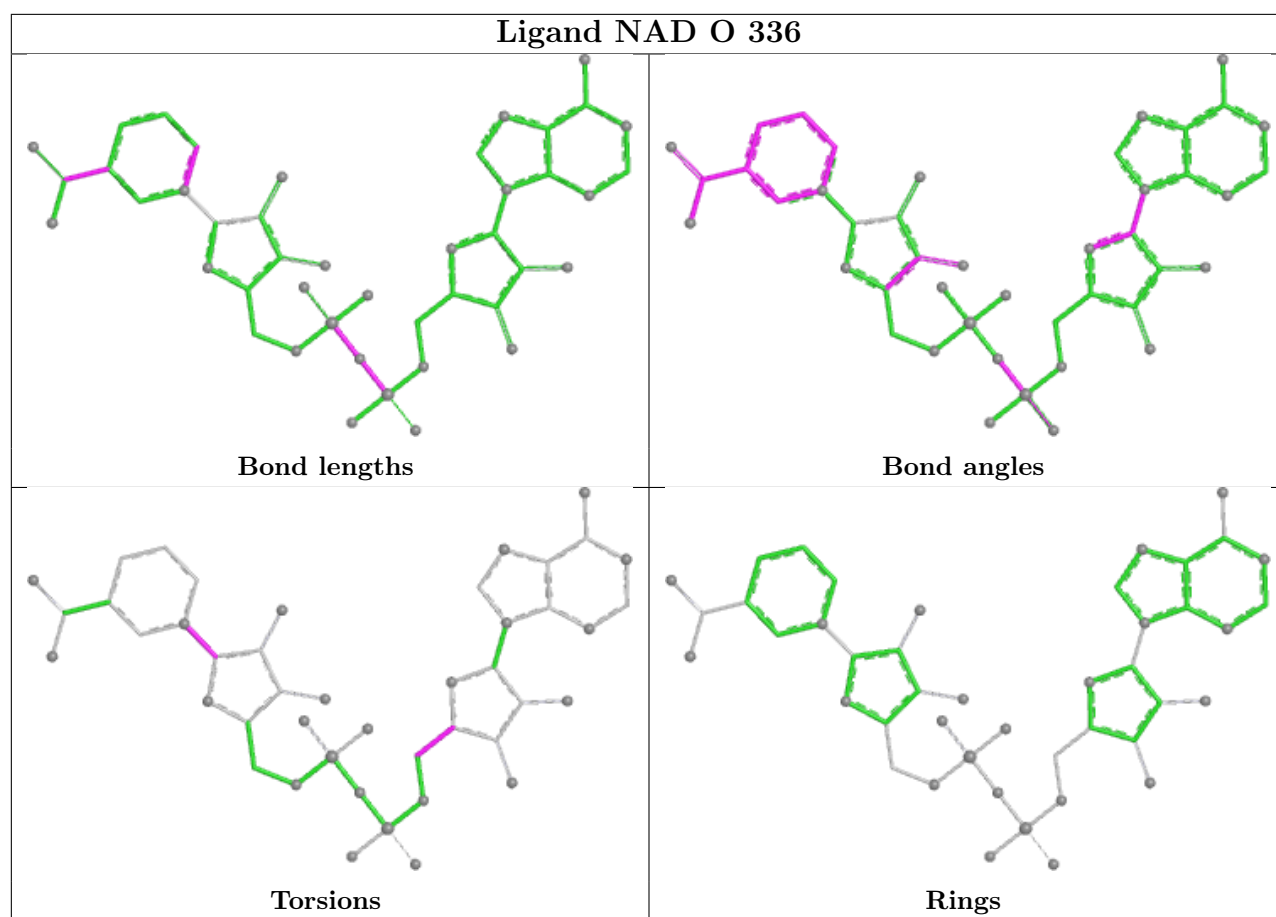
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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(Å ²)	Q<0.9
1	O	334/334 (100%)	-0.16	7 (2%) 63 64	4, 14, 37, 55	0
1	P	334/334 (100%)	-0.12	5 (1%) 72 72	3, 15, 37, 52	0
1	Q	334/334 (100%)	-0.02	14 (4%) 40 40	4, 16, 43, 59	0
1	R	334/334 (100%)	-0.19	5 (1%) 72 72	4, 14, 34, 60	0
All	All	1336/1336 (100%)	-0.12	31 (2%) 61 61	3, 15, 38, 60	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	61	GLY	4.9
1	Q	23	PRO	3.6
1	Q	68	GLY	3.3
1	Q	0	ALA	3.1
1	O	62	ASN	3.1
1	O	0	ALA	3.0
1	P	23	PRO	2.9
1	Q	332	GLY	2.8
1	Q	265	GLY	2.6
1	O	78	ASP	2.6
1	P	0	ALA	2.6
1	P	60	ASN	2.6
1	O	60	ASN	2.6
1	Q	249	GLU	2.5
1	O	38	ASN	2.4
1	P	86	GLU	2.4
1	Q	25	ILE	2.4
1	Q	300	ILE	2.4
1	Q	333	LEU	2.4
1	Q	21	LYS	2.3
1	R	62	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	80	GLU	2.2
1	R	220	GLU	2.2
1	R	0	ALA	2.2
1	O	247	GLU	2.2
1	Q	266	GLU	2.1
1	R	78	ASP	2.1
1	Q	22	ASN	2.1
1	R	98	ARG	2.0
1	Q	253	GLU	2.0
1	Q	60	ASN	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](#)

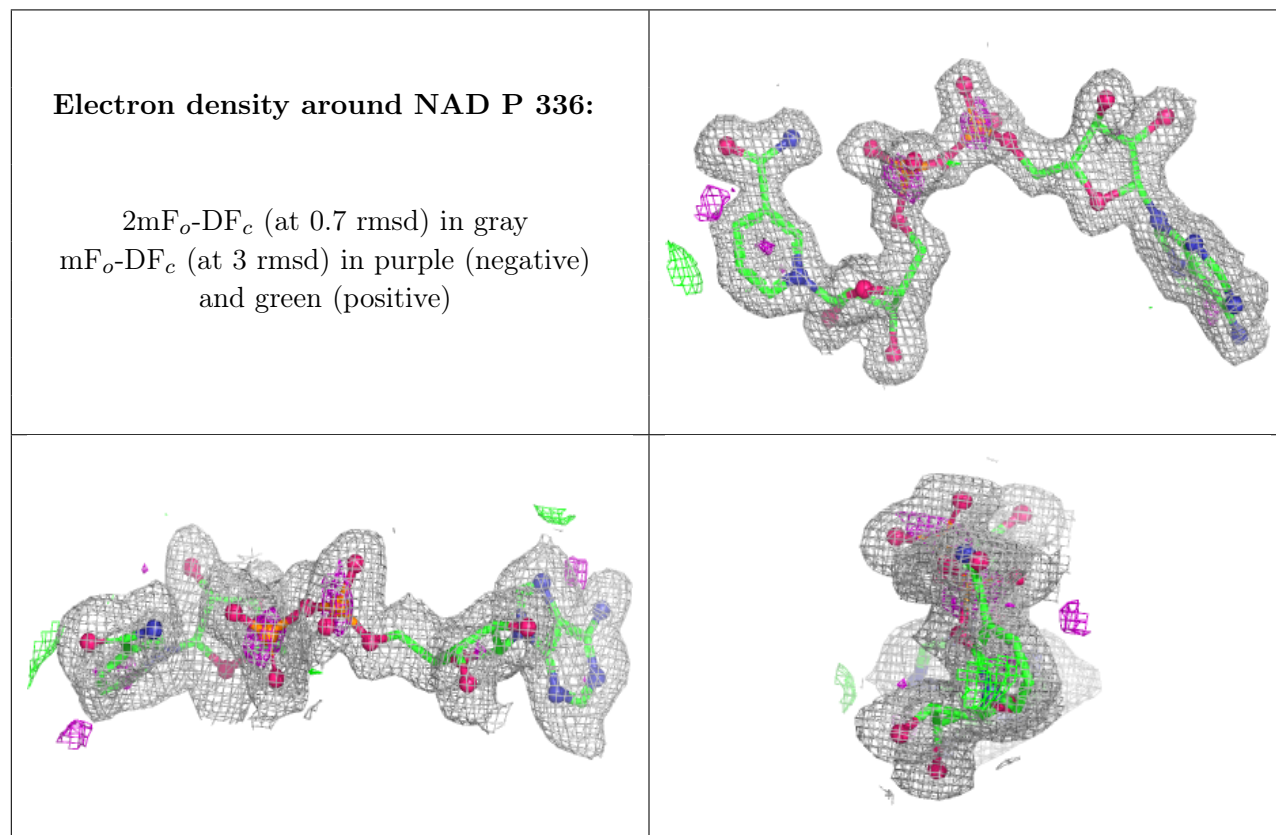
There are no oligosaccharides in this entry.

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.

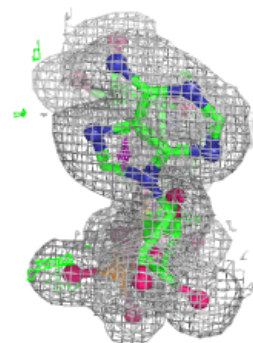
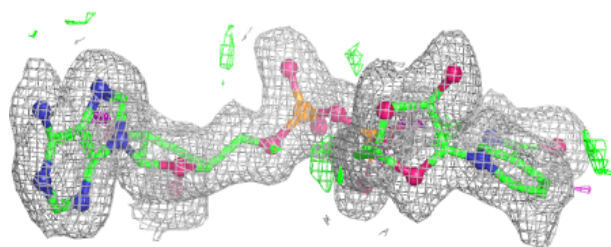
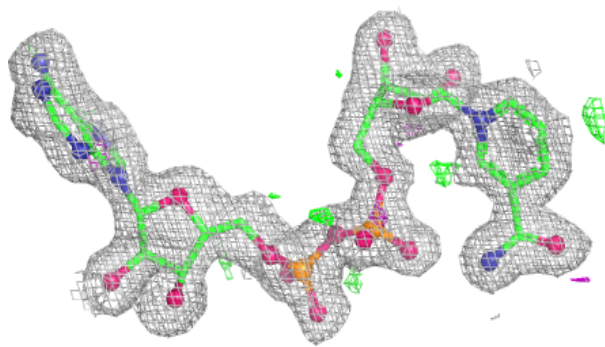
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	R	339	5/5	0.85	0.20	26,27,32,38	0
2	SO4	Q	339	5/5	0.91	0.21	27,28,32,34	0
2	SO4	O	339	5/5	0.92	0.23	23,26,35,37	0
2	SO4	P	339	5/5	0.92	0.18	30,31,34,36	0
2	SO4	O	338	5/5	0.94	0.13	17,18,19,20	0
2	SO4	Q	338	5/5	0.94	0.11	20,24,26,28	0
2	SO4	R	338	5/5	0.96	0.14	23,26,33,33	0
2	SO4	P	338	5/5	0.96	0.15	33,35,39,40	0
3	NAD	P	336	44/44	0.97	0.06	4,10,12,17	0
3	NAD	R	336	44/44	0.97	0.05	7,11,16,18	0
3	NAD	Q	336	44/44	0.98	0.05	2,10,12,13	0
3	NAD	O	336	44/44	0.98	0.05	5,9,16,19	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.

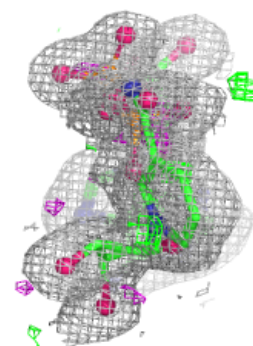
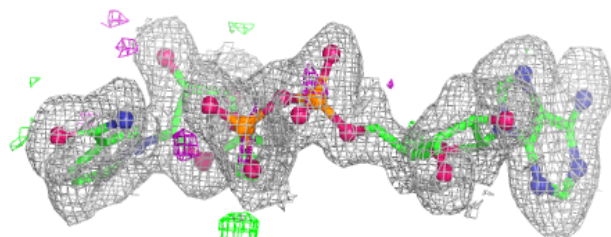
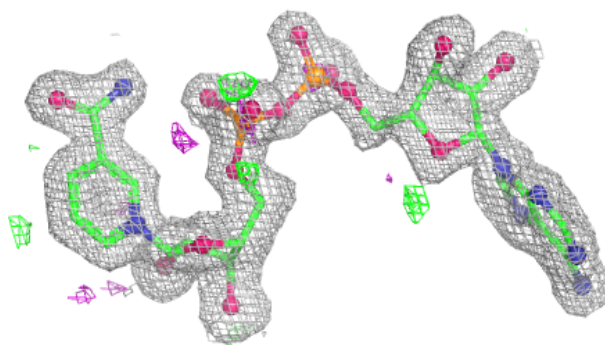


Electron density around NAD R 336:

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

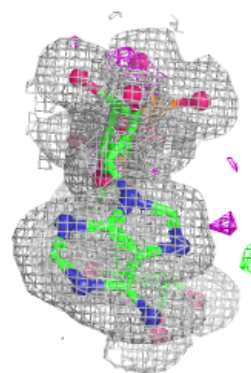
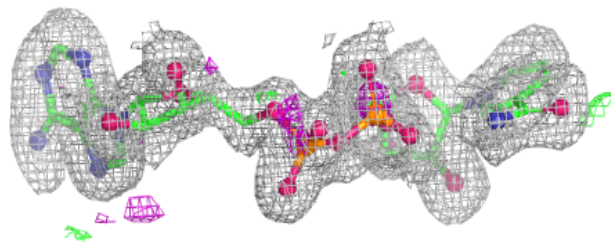
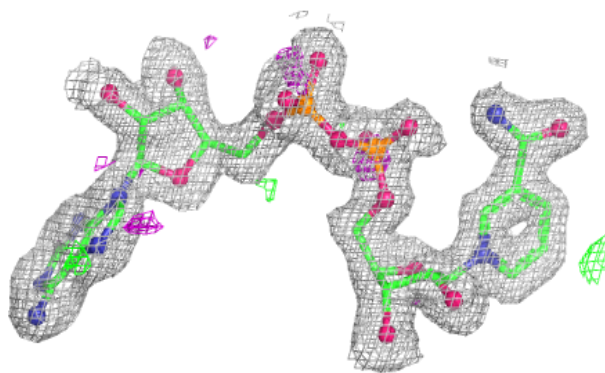
**Electron density around NAD Q 336:**

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



Electron density around NAD O 336:

$2mF_o-DF_c$ (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.