



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 10:58 PM EDT

PDB ID : 3KSZ  
Title : Crystal Structure of C151S+H178N mutant of Glyceraldehyde-3-phosphate-dehydrogenase 1 (GAPDH 1) from Staphylococcus aureus MRSA252 complexed with NAD and G3P  
Authors : Mukherjee, S.; Dutta, D.; Saha, B.; Das, A.K.  
Deposited on : 2009-11-24  
Resolution : 2.60 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](mailto: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.

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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 : 2.23.2  
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) : 2.23.2

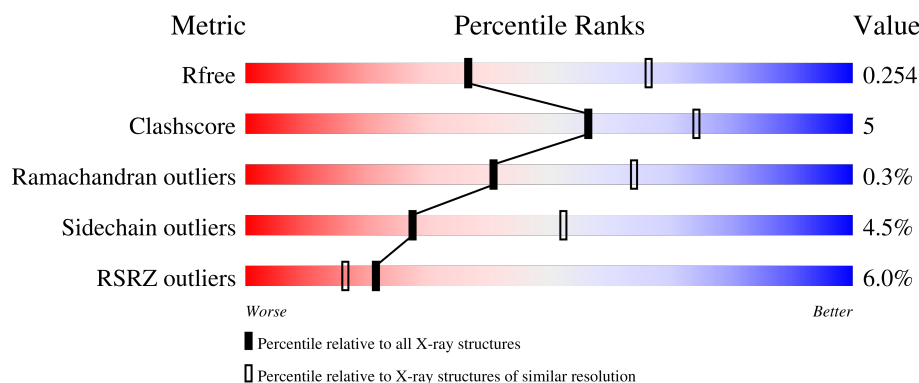
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	336	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	P	336	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>
1	Q	336	<div> <div>10%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	R	336	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10424 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 Glyceraldehyde-3-phosphate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2527	1572	434	513	8			
1	P	334	Total	C	N	O	S	0	0	0
			2527	1572	434	513	8			
1	R	334	Total	C	N	O	S	0	0	0
			2527	1572	434	513	8			
1	Q	333	Total	C	N	O	S	0	1	0
			2524	1571	433	512	8			

There are 8 discrepancies between the modelled and reference sequences:

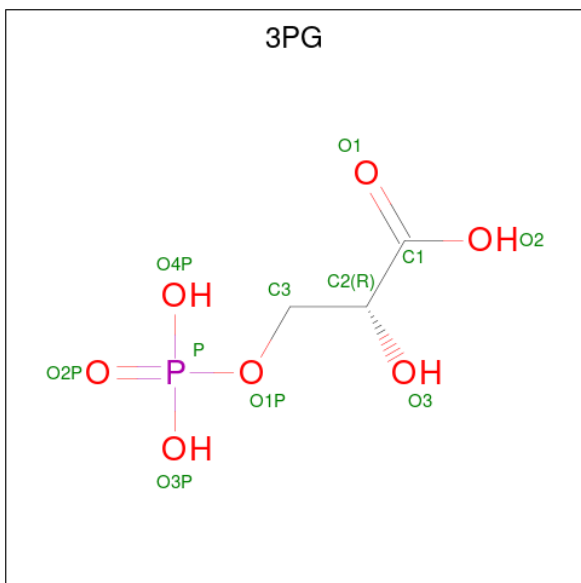
Chain	Residue	Modelled	Actual	Comment	Reference
O	151	SER	CYS	engineered mutation	UNP Q6GIL8
O	178	ASN	HIS	engineered mutation	UNP Q6GIL8
P	151	SER	CYS	engineered mutation	UNP Q6GIL8
P	178	ASN	HIS	engineered mutation	UNP Q6GIL8
R	151	SER	CYS	engineered mutation	UNP Q6GIL8
R	178	ASN	HIS	engineered mutation	UNP Q6GIL8
Q	151	SER	CYS	engineered mutation	UNP Q6GIL8
Q	178	ASN	HIS	engineered mutation	UNP Q6GIL8

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	P	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	R	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula:  $\text{C}_3\text{H}_7\text{O}_7\text{P}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	O	P	0	0
			10	3	6	1		
3	P	1	Total	C	O	P	0	0
			11	3	7	1		
3	R	1	Total	C	O	P	0	0
			10	3	6	1		
3	Q	1	Total	C	O	P	0	0
			11	3	7	1		

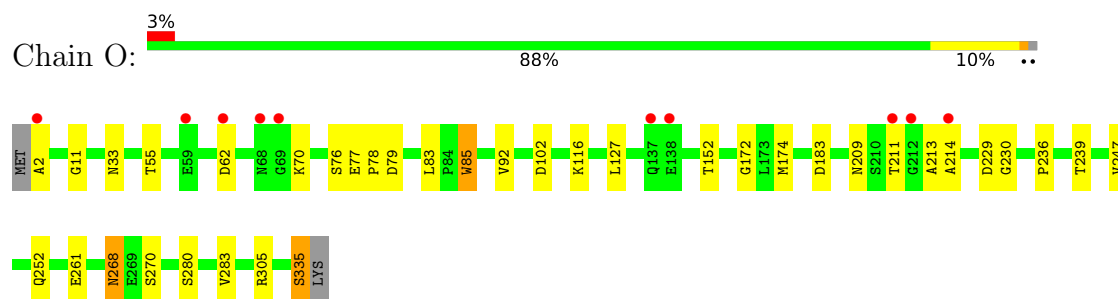
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	26	Total	O	0	0
			26	26		
4	P	32	Total	O	0	0
			32	32		
4	R	18	Total	O	0	0
			18	18		
4	Q	25	Total	O	0	0
			25	25		

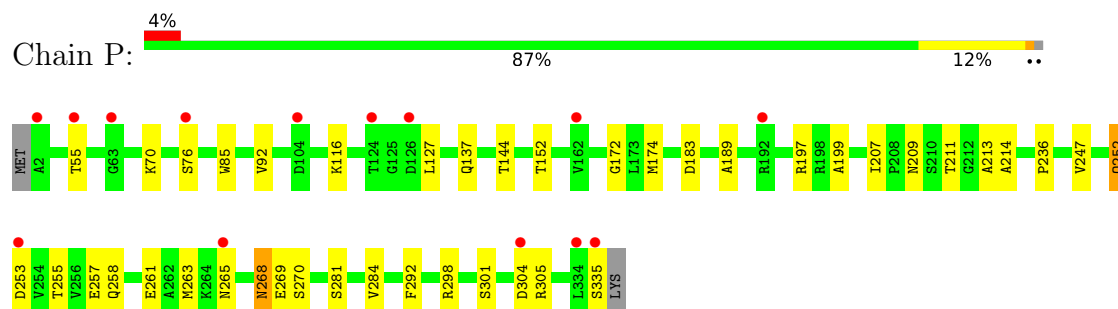
### 3 Residue-property plots

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.

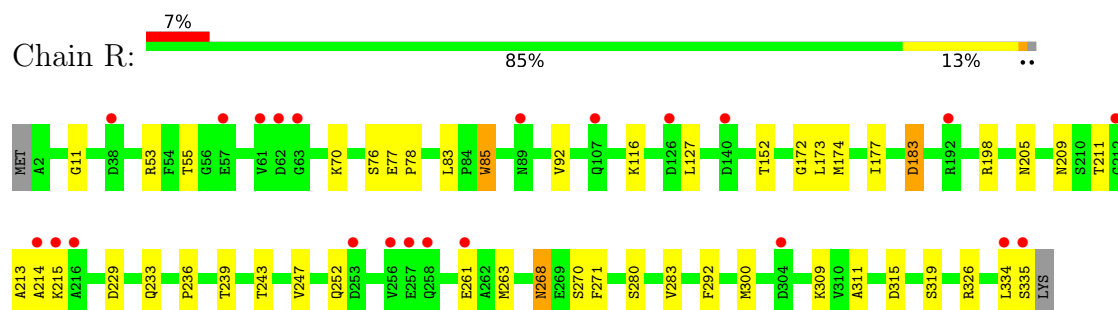
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



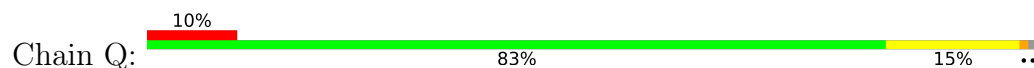
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1

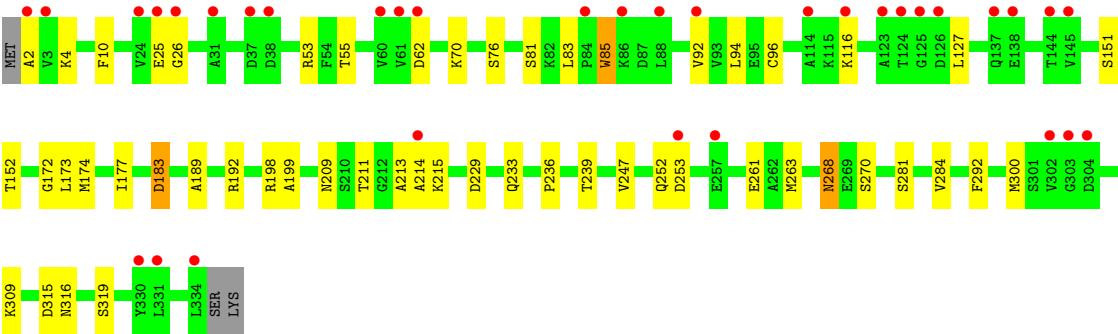


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.87Å 93.60Å 89.88Å 90.00° 107.61° 90.00°	Depositor
Resolution (Å)	33.83 – 2.60 33.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.83-2.60) 99.0 (33.83-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.200 , 0.248 0.214 , 0.254	Depositor DCC
$R_{free}$ test set	1657 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: 3PG, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	O	0.67	0/2560	0.74	0/3469
1	P	0.67	0/2560	0.71	0/3469
1	Q	0.60	0/2560	0.66	0/3469
1	R	0.63	0/2560	0.68	0/3469
All	All	0.64	0/10240	0.70	0/13876

There are no bond length outliers.

There are no bond angle outliers.

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	2527	0	2504	22	4
1	P	2527	0	2504	30	2
1	Q	2524	0	2504	35	8
1	R	2527	0	2504	29	6
2	O	44	0	26	2	0
2	P	44	0	26	0	0
2	Q	44	0	26	2	0
2	R	44	0	26	1	0
3	O	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	11	0	5	0	0
3	Q	11	0	5	0	0
3	R	10	0	4	0	0
4	O	26	0	0	4	0
4	P	32	0	0	9	0
4	Q	25	0	0	10	0
4	R	18	0	0	3	0
All	All	10424	0	10138	103	10

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (103) 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:P:265:ASN:HB3	4:P:345:HOH:O	1.55	1.06
1:Q:198:ARG:HD3	4:Q:339:HOH:O	1.55	1.04
1:P:257:GLU:HG3	4:P:343:HOH:O	1.66	0.92
1:O:2:ALA:HA	4:O:338:HOH:O	1.71	0.90
1:Q:215:LYS:HB2	4:Q:357:HOH:O	1.78	0.81
1:P:269:GLU:HG3	4:P:347:HOH:O	1.83	0.78
1:P:137:GLN:HG2	4:P:338:HOH:O	1.83	0.76
1:Q:2:ALA:HB3	4:Q:354:HOH:O	1.91	0.70
1:Q:309:LYS:HD3	4:Q:341:HOH:O	1.92	0.69
1:O:305:ARG:HH21	1:P:305:ARG:HH21	1.41	0.67
4:O:358:HOH:O	1:P:298:ARG:HD3	1.96	0.66
1:O:116:LYS:CE	1:O:335:SER:HB3	2.27	0.65
1:P:257:GLU:HB2	4:P:349:HOH:O	1.95	0.64
1:R:173:LEU:HD13	1:Q:309:LYS:HB2	1.80	0.63
1:R:152:THR:HB	1:R:213:ALA:HB2	1.80	0.63
1:O:152:THR:HB	1:O:213:ALA:HB2	1.80	0.62
1:Q:192:ARG:HG3	4:Q:360:HOH:O	2.00	0.61
1:P:137:GLN:CG	4:P:338:HOH:O	2.44	0.61
1:P:268:ASN:HD22	1:P:270:SER:H	1.50	0.60
1:P:144:THR:HG22	4:P:342:HOH:O	2.00	0.60
1:R:53:ARG:HG3	4:R:346:HOH:O	2.00	0.60
1:O:92:VAL:HG22	1:O:116:LYS:HB2	1.83	0.59
1:Q:92:VAL:HG22	1:Q:116:LYS:HB2	1.85	0.58
1:R:309:LYS:HB2	1:Q:173:LEU:HD13	1.85	0.58
1:O:305:ARG:NH2	1:P:305:ARG:HH21	2.01	0.58
1:P:152:THR:HB	1:P:213:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:177:ILE:HD13	1:Q:233:GLN:HG3	1.86	0.57
1:R:334:LEU:HD21	4:R:353:HOH:O	2.05	0.57
1:P:255:THR:OG1	1:P:258:GLN:HG3	2.05	0.56
1:O:83:LEU:HD13	1:O:85:TRP:CZ2	2.41	0.56
1:R:315:ASP:O	1:R:319:SER:HB2	2.07	0.55
1:P:268:ASN:ND2	1:P:270:SER:H	2.05	0.55
1:R:92:VAL:HG22	1:R:116:LYS:HB2	1.89	0.55
1:O:11:GLY:HA3	2:O:0:NAD:O5B	2.08	0.54
1:R:172:GLY:HA3	1:R:247:VAL:HG12	1.90	0.54
1:O:33:ASN:ND2	2:O:0:NAD:H2A	2.23	0.54
1:R:268:ASN:ND2	1:R:270:SER:H	2.06	0.53
1:R:11:GLY:HA3	2:R:0:NAD:O5B	2.08	0.52
1:O:236:PRO:HB2	1:P:236:PRO:HB2	1.91	0.52
1:Q:4:LYS:HE3	4:Q:354:HOH:O	2.10	0.51
1:R:53:ARG:CG	4:R:346:HOH:O	2.57	0.51
1:O:116:LYS:HE3	1:O:335:SER:HB3	1.93	0.50
1:R:300:MET:CE	1:Q:229:ASP:HB2	2.42	0.50
1:P:268:ASN:HD22	1:P:270:SER:N	2.10	0.50
1:R:236:PRO:HB2	1:Q:236:PRO:HB2	1.94	0.49
1:R:268:ASN:HD22	1:R:270:SER:H	1.60	0.49
1:P:116:LYS:HE2	1:P:335:SER:HB2	1.94	0.49
1:Q:174:MET:CE	1:Q:211:THR:HG21	2.43	0.49
1:O:305:ARG:HH21	1:P:305:ARG:NH2	2.09	0.49
1:O:305:ARG:NH2	1:P:305:ARG:NH2	2.60	0.49
1:Q:152:THR:HB	1:Q:213:ALA:HB2	1.95	0.49
1:Q:151[B]:SER:OG	2:Q:0:NAD:H4N	2.13	0.48
1:Q:81:SER:HB2	4:Q:346:HOH:O	2.13	0.48
1:Q:263:MET:HG3	1:Q:292:PHE:CE1	2.49	0.47
1:P:197:ARG:HB3	1:P:207:ILE:HG23	1.97	0.47
1:R:233:GLN:HG3	1:Q:177:ILE:HD13	1.96	0.47
1:P:174:MET:CE	1:P:211:THR:HG21	2.45	0.47
1:Q:268:ASN:ND2	1:Q:270:SER:H	2.13	0.46
1:Q:309:LYS:CD	4:Q:341:HOH:O	2.60	0.46
1:P:92:VAL:HG22	1:P:116:LYS:HB2	1.98	0.45
1:Q:189:ALA:O	1:Q:199:ALA:HB1	2.16	0.45
1:R:280:SER:O	1:R:283:VAL:HG22	2.16	0.45
1:R:334:LEU:O	1:R:335:SER:HB3	2.16	0.45
1:R:268:ASN:ND2	1:R:271:PHE:H	2.15	0.45
1:Q:183:ASP:OD2	1:Q:198:ARG:NH1	2.50	0.45
1:O:116:LYS:HE2	1:O:335:SER:HB3	1.98	0.45
1:Q:25:GLU:HG2	1:Q:26:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:252:GLN:HG2	1:P:304:ASP:O	2.18	0.44
1:R:77:GLU:HA	1:R:78:PRO:HD3	1.85	0.44
1:P:257:GLU:CB	4:P:349:HOH:O	2.59	0.43
1:R:229:ASP:HB2	1:Q:300:MET:CE	2.48	0.43
1:Q:268:ASN:HD22	1:Q:270:SER:H	1.66	0.43
1:O:280:SER:O	1:O:283:VAL:HG22	2.18	0.43
1:R:183:ASP:OD2	1:R:198:ARG:NH1	2.52	0.43
1:O:77:GLU:HA	1:O:78:PRO:HD3	1.85	0.43
1:R:174:MET:CE	1:R:211:THR:HG21	2.48	0.43
1:O:174:MET:HE1	1:O:211:THR:HG21	2.01	0.43
1:P:172:GLY:HA3	1:P:247:VAL:HG12	2.00	0.43
1:P:281:SER:HA	1:P:284:VAL:HG23	2.01	0.43
1:R:268:ASN:HD22	1:R:271:PHE:H	1.66	0.43
1:Q:96:CYS:O	2:Q:0:NAD:H51N	2.19	0.43
1:Q:53:ARG:NH2	4:Q:348:HOH:O	2.53	0.42
1:Q:281:SER:HA	1:Q:284:VAL:HG23	2.01	0.42
1:O:174:MET:CE	1:O:211:THR:HG21	2.49	0.42
1:P:116:LYS:HE3	1:P:335:SER:HB3	2.00	0.42
1:P:263:MET:HG3	1:P:292:PHE:CE1	2.54	0.42
1:O:229:ASP:HB3	4:O:358:HOH:O	2.19	0.42
1:R:263:MET:HG3	1:R:292:PHE:CE1	2.55	0.41
1:Q:315:ASP:O	1:Q:319:SER:HB2	2.20	0.41
1:Q:172:GLY:HA3	1:Q:247:VAL:HG12	2.03	0.41
1:R:243:THR:O	1:R:311:ALA:HA	2.20	0.41
1:R:205:ASN:HD22	1:Q:281:SER:H	1.67	0.41
1:R:263:MET:HG3	1:R:292:PHE:CZ	2.56	0.41
1:Q:83:LEU:HD13	1:Q:85:TRP:CZ2	2.55	0.41
1:Q:174:MET:HE1	1:Q:211:THR:HG21	2.02	0.41
1:O:172:GLY:HA3	1:O:247:VAL:HG12	2.01	0.41
1:Q:62:ASP:HB3	4:Q:359:HOH:O	2.21	0.41
1:Q:94:LEU:HD23	1:Q:94:LEU:HA	1.89	0.41
1:O:268:ASN:ND2	1:O:270:SER:H	2.19	0.40
1:R:83:LEU:HD13	1:R:85:TRP:CZ2	2.57	0.40
1:P:189:ALA:O	1:P:199:ALA:HB1	2.21	0.40
1:P:255:THR:HA	4:P:339:HOH:O	2.20	0.40
1:O:230:GLY:N	4:O:358:HOH:O	2.53	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:326:ARG:NE	1:Q:25:GLU:CG[1_455]	1.73	0.47
1:R:326:ARG:NE	1:Q:25:GLU:CD[1_455]	1.84	0.36
1:R:326:ARG:CZ	1:Q:25:GLU:OE2[1_455]	1.88	0.32
1:O:62:ASP:CB	1:Q:215:LYS:CB[2_656]	1.91	0.29
1:R:326:ARG:NE	1:Q:25:GLU:OE2[1_455]	1.95	0.25
1:O:79:ASP:OD2	1:P:265:ASN:OD1[2_555]	2.00	0.20
1:O:102:ASP:OD1	1:P:269:GLU:OE1[2_555]	2.04	0.16
1:O:62:ASP:OD1	1:Q:215:LYS:O[2_656]	2.07	0.13
1:R:326:ARG:CD	1:Q:25:GLU:CD[1_455]	2.07	0.13
1:R:215:LYS:NZ	1:Q:81:SER:O[2_656]	2.18	0.02

## 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	332/336 (99%)	312 (94%)	19 (6%)	1 (0%)	41	64
1	P	332/336 (99%)	314 (95%)	17 (5%)	1 (0%)	41	64
1	Q	332/336 (99%)	313 (94%)	18 (5%)	1 (0%)	41	64
1	R	332/336 (99%)	311 (94%)	20 (6%)	1 (0%)	41	64
All	All	1328/1344 (99%)	1250 (94%)	74 (6%)	4 (0%)	41	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	214	ALA
1	O	214	ALA
1	P	214	ALA
1	Q	214	ALA

### 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	272/274 (99%)	260 (96%)	12 (4%)	28	53
1	P	272/274 (99%)	260 (96%)	12 (4%)	28	53
1	Q	272/274 (99%)	258 (95%)	14 (5%)	24	46
1	R	272/274 (99%)	261 (96%)	11 (4%)	31	57
All	All	1088/1096 (99%)	1039 (96%)	49 (4%)	27	52

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

Mol	Chain	Res	Type
1	O	55	THR
1	O	70	LYS
1	O	76	SER
1	O	85	TRP
1	O	127	LEU
1	O	183	ASP
1	O	209	ASN
1	O	239	THR
1	O	252	GLN
1	O	261	GLU
1	O	268	ASN
1	O	335	SER
1	P	55	THR
1	P	70	LYS
1	P	76	SER
1	P	85	TRP
1	P	127	LEU
1	P	183	ASP
1	P	209	ASN
1	P	252	GLN
1	P	253	ASP
1	P	261	GLU
1	P	268	ASN
1	P	301	SER

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Mol	Chain	Res	Type
1	R	55	THR
1	R	70	LYS
1	R	76	SER
1	R	85	TRP
1	R	127	LEU
1	R	183	ASP
1	R	209	ASN
1	R	239	THR
1	R	252	GLN
1	R	261	GLU
1	R	268	ASN
1	Q	10	PHE
1	Q	55	THR
1	Q	70	LYS
1	Q	76	SER
1	Q	85	TRP
1	Q	127	LEU
1	Q	183	ASP
1	Q	209	ASN
1	Q	239	THR
1	Q	252	GLN
1	Q	253	ASP
1	Q	261	GLU
1	Q	268	ASN
1	Q	316	ASN

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	68	ASN
1	O	205	ASN
1	O	265	ASN
1	O	268	ASN
1	O	296	GLN
1	P	68	ASN
1	P	205	ASN
1	P	265	ASN
1	P	268	ASN
1	P	296	GLN
1	R	68	ASN
1	R	205	ASN
1	R	265	ASN

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Mol	Chain	Res	Type
1	R	268	ASN
1	R	296	GLN
1	Q	178	ASN
1	Q	205	ASN
1	Q	265	ASN
1	Q	268	ASN
1	Q	296	GLN
1	Q	316	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	3PG	P	337	-	7,10,10	2.58	4 (57%)	10,14,14	2.05	3 (30%)
3	3PG	Q	337	-	7,10,10	3.06	4 (57%)	10,14,14	2.22	4 (40%)
2	NAD	R	0	-	42,48,48	1.73	6 (14%)	50,73,73	1.70	8 (16%)
2	NAD	P	0	-	42,48,48	1.82	6 (14%)	50,73,73	1.75	8 (16%)
3	3PG	O	337	-	8,9,10	2.15	3 (37%)	10,12,14	1.73	4 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	3PG	R	337	-	8,9,10	2.51	3 (37%)	10,12,14	1.83	3 (30%)
2	NAD	O	0	-	42,48,48	1.90	5 (11%)	50,73,73	1.52	7 (14%)
2	NAD	Q	0	-	42,48,48	1.78	4 (9%)	50,73,73	1.46	10 (20%)

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	3PG	P	337	-	-	1/6/10/10	-
3	3PG	Q	337	-	-	4/6/10/10	-
2	NAD	R	0	-	-	5/26/62/62	0/5/5/5
2	NAD	P	0	-	-	7/26/62/62	0/5/5/5
3	3PG	O	337	-	-	3/7/8/10	-
3	3PG	R	337	-	-	5/7/8/10	-
2	NAD	O	0	-	-	6/26/62/62	0/5/5/5
2	NAD	Q	0	-	-	10/26/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	0	NAD	O7N-C7N	9.15	1.41	1.24
2	P	0	NAD	O7N-C7N	8.31	1.40	1.24
2	Q	0	NAD	O7N-C7N	8.07	1.39	1.24
2	R	0	NAD	O7N-C7N	7.50	1.38	1.24
3	Q	337	3PG	P-O1P	5.42	1.77	1.60
2	Q	0	NAD	C2A-N3A	4.73	1.39	1.32
2	O	0	NAD	C2A-N3A	4.42	1.39	1.32
3	P	337	3PG	P-O1P	4.19	1.73	1.60
3	R	337	3PG	C3-C2	4.13	1.57	1.51
3	R	337	3PG	P-O2P	4.01	1.63	1.50
2	R	0	NAD	C2A-N3A	3.83	1.38	1.32
3	Q	337	3PG	P-O2P	3.48	1.61	1.50
2	R	0	NAD	C2N-N1N	3.43	1.39	1.35
2	Q	0	NAD	C2N-N1N	3.36	1.39	1.35
3	O	337	3PG	C3-C2	3.35	1.56	1.51
2	P	0	NAD	C2A-N3A	3.31	1.37	1.32
3	O	337	3PG	P-O2P	3.21	1.60	1.50
3	Q	337	3PG	C3-C2	3.05	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	337	3PG	P-O2P	3.04	1.60	1.50
3	R	337	3PG	P-O1P	2.97	1.69	1.60
3	O	337	3PG	P-O1P	2.93	1.69	1.60
2	P	0	NAD	O4D-C1D	2.93	1.45	1.41
2	P	0	NAD	C2N-N1N	2.87	1.38	1.35
3	P	337	3PG	O1P-C3	2.74	1.55	1.44
3	Q	337	3PG	O1P-C3	2.74	1.55	1.44
3	P	337	3PG	C3-C2	2.70	1.60	1.50
2	R	0	NAD	C2A-N1A	2.59	1.38	1.33
2	O	0	NAD	C2B-C1B	-2.51	1.50	1.53
2	P	0	NAD	C2A-N1A	2.44	1.38	1.33
2	O	0	NAD	C2N-N1N	2.41	1.37	1.35
2	Q	0	NAD	O4B-C4B	-2.32	1.39	1.45
2	R	0	NAD	O4B-C4B	-2.22	1.40	1.45
2	R	0	NAD	C8A-N7A	2.06	1.38	1.34
2	O	0	NAD	C3N-C7N	2.02	1.53	1.50
2	P	0	NAD	C7N-N7N	2.01	1.36	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	0	NAD	N3A-C2A-N1A	-7.14	117.51	128.68
2	P	0	NAD	O7N-C7N-C3N	-5.97	112.49	119.63
2	O	0	NAD	N3A-C2A-N1A	-5.88	119.49	128.68
2	P	0	NAD	N3A-C2A-N1A	-5.27	120.43	128.68
2	Q	0	NAD	N3A-C2A-N1A	-4.59	121.51	128.68
2	O	0	NAD	C3N-C7N-N7N	4.10	122.67	117.75
3	Q	337	3PG	P-O1P-C3	3.99	129.27	118.30
2	P	0	NAD	C3N-C7N-N7N	3.85	122.37	117.75
3	P	337	3PG	P-O1P-C3	3.77	128.68	118.30
2	O	0	NAD	O7N-C7N-C3N	-3.55	115.38	119.63
2	R	0	NAD	PN-O3-PA	-3.50	120.81	132.83
3	Q	337	3PG	O1P-C3-C2	3.39	117.72	107.94
3	Q	337	3PG	O3P-P-O1P	3.30	115.52	106.73
3	P	337	3PG	O4P-P-O1P	3.28	115.47	106.73
2	Q	0	NAD	C3N-C7N-N7N	3.25	121.65	117.75
3	R	337	3PG	O3P-P-O1P	3.15	115.11	106.73
3	O	337	3PG	P-O1P-C3	3.10	126.83	118.30
3	O	337	3PG	O3P-P-O1P	3.09	114.95	106.73
3	R	337	3PG	O1P-C3-C2	3.05	116.42	108.33
2	Q	0	NAD	PN-O3-PA	-3.05	122.35	132.83
3	P	337	3PG	O1P-C3-C2	2.98	116.54	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	0	NAD	C6N-N1N-C2N	-2.96	119.28	121.97
2	R	0	NAD	O3D-C3D-C2D	-2.71	103.05	111.82
2	O	0	NAD	C4A-C5A-N7A	-2.65	106.64	109.40
3	Q	337	3PG	O4P-P-O2P	-2.64	100.34	110.68
2	P	0	NAD	O5B-C5B-C4B	-2.58	100.11	108.99
2	Q	0	NAD	O2N-PN-O1N	2.58	124.97	112.24
2	O	0	NAD	C1B-N9A-C4A	-2.55	122.16	126.64
2	R	0	NAD	C3N-C7N-N7N	2.40	120.63	117.75
2	P	0	NAD	C1B-N9A-C4A	-2.38	122.47	126.64
2	R	0	NAD	O4D-C1D-C2D	-2.35	103.49	106.93
2	Q	0	NAD	O5B-C5B-C4B	-2.34	100.92	108.99
2	O	0	NAD	O3B-C3B-C4B	-2.34	104.28	111.05
2	R	0	NAD	C1B-N9A-C4A	-2.33	122.54	126.64
3	O	337	3PG	O1P-C3-C2	2.29	114.41	108.33
2	Q	0	NAD	C4A-C5A-N7A	-2.26	107.04	109.40
2	Q	0	NAD	O3B-C3B-C4B	-2.23	104.61	111.05
2	P	0	NAD	C2N-N1N-C1D	2.21	124.05	119.14
3	R	337	3PG	P-O1P-C3	2.16	124.25	118.30
2	R	0	NAD	O7N-C7N-C3N	-2.15	117.06	119.63
2	P	0	NAD	O2D-C2D-C1D	-2.15	102.90	110.85
2	Q	0	NAD	O7N-C7N-C3N	-2.14	117.07	119.63
2	Q	0	NAD	O4B-C1B-C2B	-2.10	103.86	106.93
2	R	0	NAD	C4A-C5A-N7A	-2.08	107.23	109.40
2	O	0	NAD	PN-O3-PA	-2.07	125.74	132.83
2	P	0	NAD	C2N-C3N-C4N	2.02	120.54	118.26
3	O	337	3PG	O4P-P-O2P	-2.00	102.84	110.68

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	0	NAD	O4D-C1D-N1N-C2N
2	O	0	NAD	O4D-C1D-N1N-C6N
2	O	0	NAD	C2D-C1D-N1N-C2N
2	O	0	NAD	C2D-C1D-N1N-C6N
2	P	0	NAD	O4D-C1D-N1N-C2N
2	P	0	NAD	O4D-C1D-N1N-C6N
2	P	0	NAD	C2D-C1D-N1N-C2N
2	P	0	NAD	C2D-C1D-N1N-C6N
2	R	0	NAD	O4D-C1D-N1N-C2N
2	R	0	NAD	O4D-C1D-N1N-C6N
2	R	0	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	R	0	NAD	C2D-C1D-N1N-C6N
2	Q	0	NAD	O4D-C1D-N1N-C2N
2	Q	0	NAD	O4D-C1D-N1N-C6N
2	Q	0	NAD	C2D-C1D-N1N-C2N
2	Q	0	NAD	C2D-C1D-N1N-C6N
3	O	337	3PG	C1-C2-C3-O1P
3	O	337	3PG	O3-C2-C3-O1P
3	P	337	3PG	O3-C2-C3-O1P
3	R	337	3PG	O1-C1-C2-C3
3	R	337	3PG	C1-C2-C3-O1P
3	R	337	3PG	O3-C2-C3-O1P
3	R	337	3PG	C3-O1P-P-O4P
3	Q	337	3PG	C3-O1P-P-O2P
3	Q	337	3PG	C3-O1P-P-O3P
3	Q	337	3PG	C3-O1P-P-O4P
3	Q	337	3PG	C1-C2-C3-O1P
2	Q	0	NAD	O4D-C4D-C5D-O5D
2	Q	0	NAD	O4B-C4B-C5B-O5B
2	Q	0	NAD	C5D-O5D-PN-O3
2	P	0	NAD	C2N-C3N-C7N-O7N
2	P	0	NAD	O4B-C4B-C5B-O5B
2	O	0	NAD	O4B-C4B-C5B-O5B
2	P	0	NAD	C2N-C3N-C7N-N7N
2	O	0	NAD	PN-O3-PA-O1A
2	Q	0	NAD	C3D-C4D-C5D-O5D
3	O	337	3PG	C3-O1P-P-O3P
3	R	337	3PG	C3-O1P-P-O3P
2	Q	0	NAD	C5D-O5D-PN-O1N
2	R	0	NAD	O4B-C4B-C5B-O5B
2	Q	0	NAD	C3B-C4B-C5B-O5B

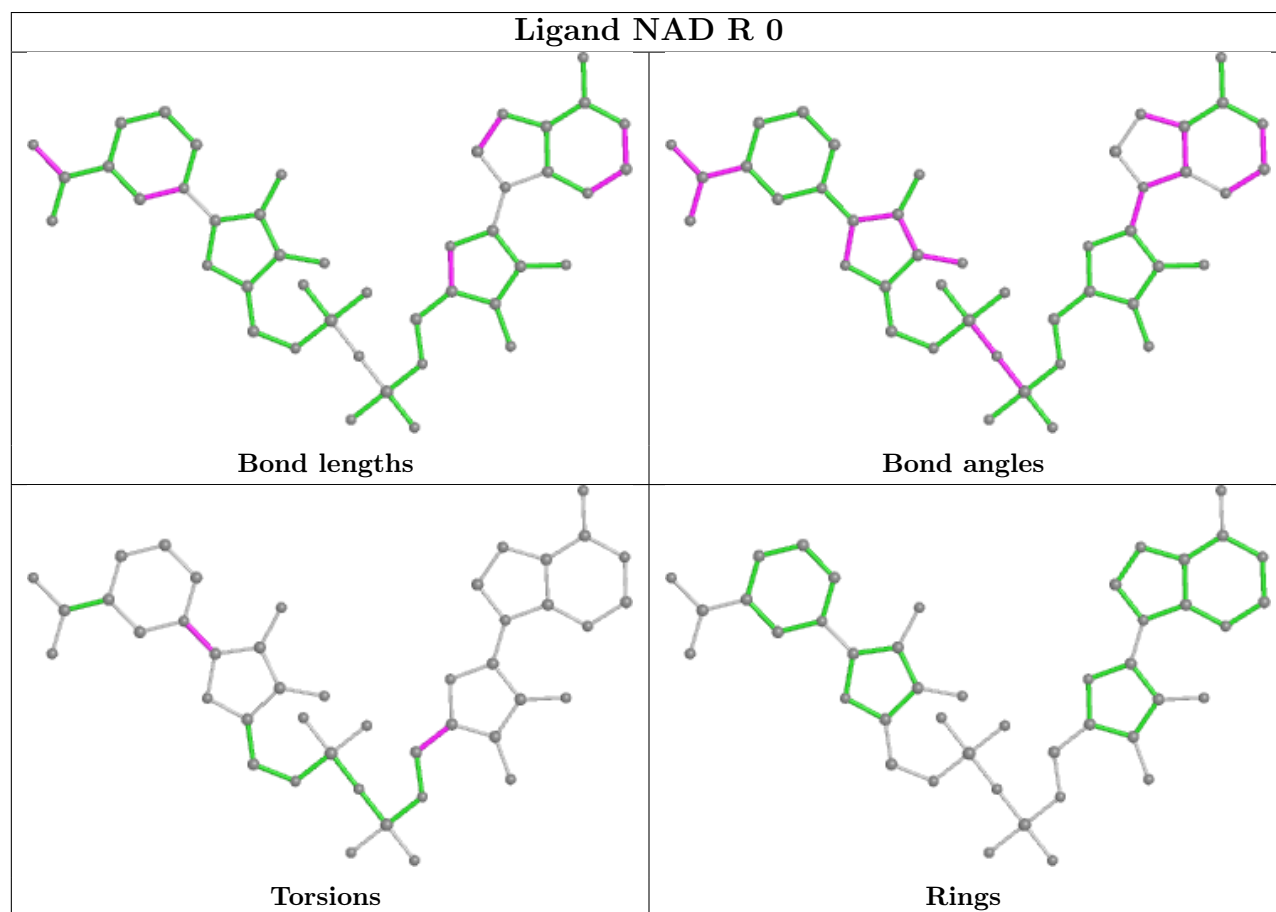
There are no ring outliers.

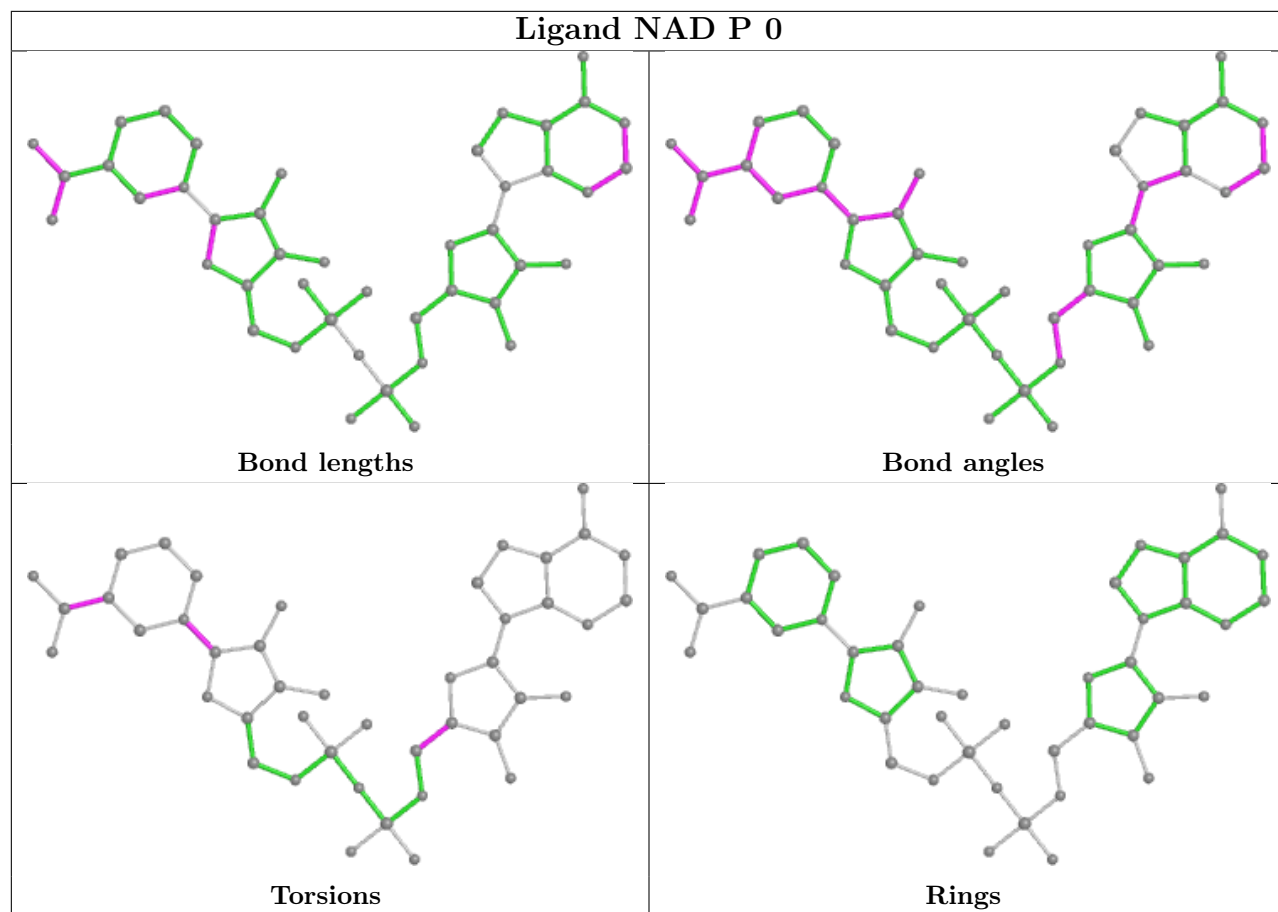
3 monomers are involved in 5 short contacts:

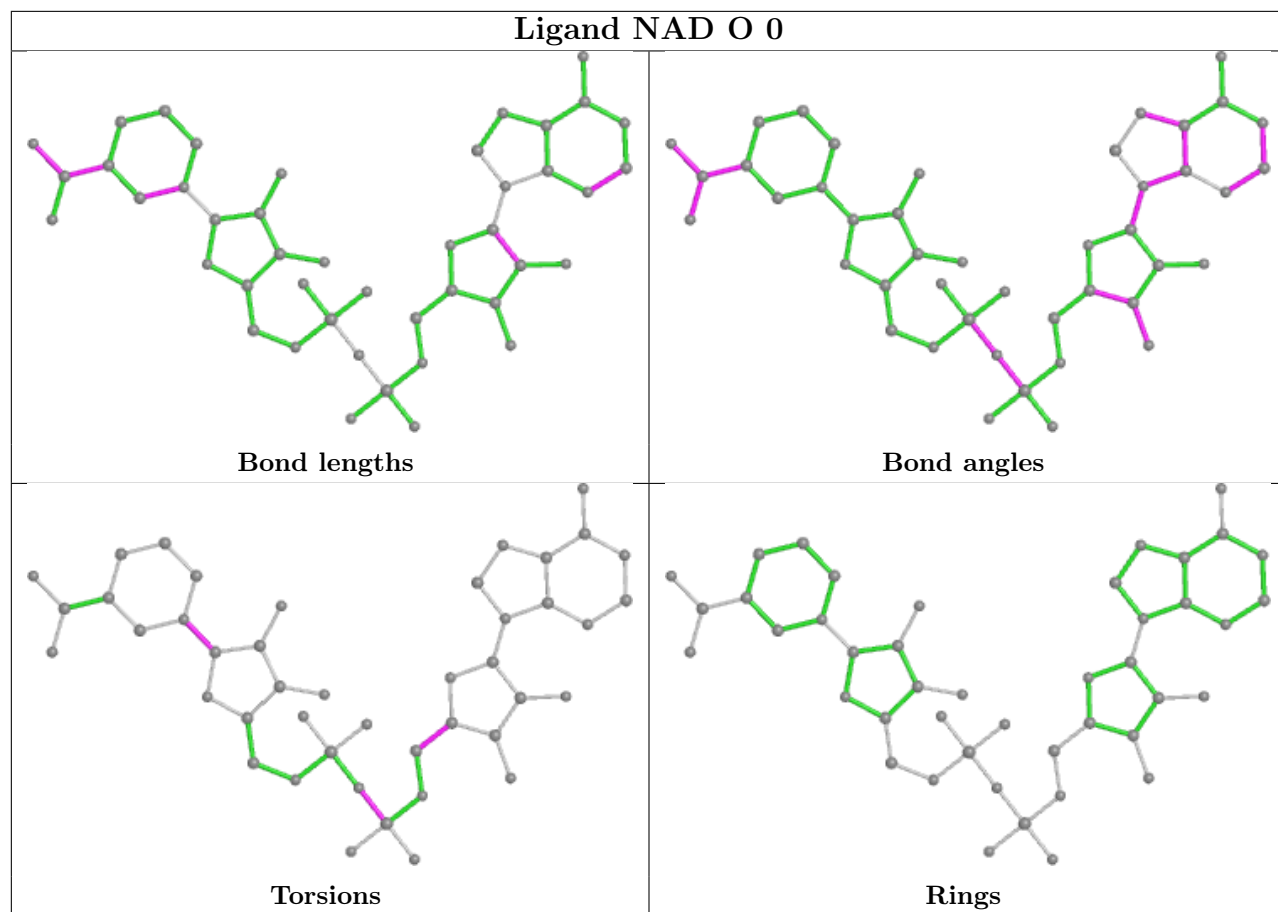
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	0	NAD	1	0
2	O	0	NAD	2	0
2	Q	0	NAD	2	0

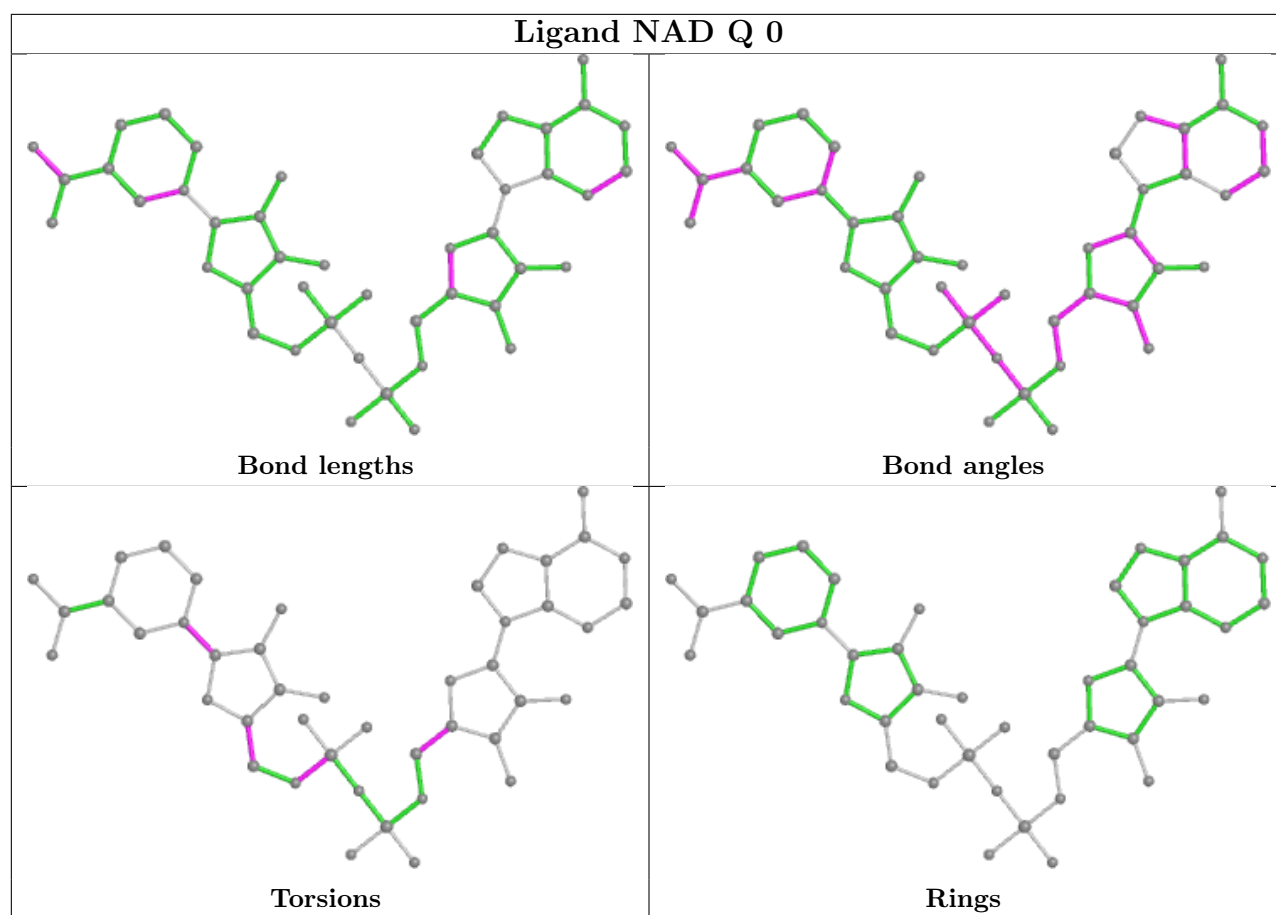
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	334/336 (99%)	0.13	10 (2%) 50 43	33, 45, 62, 72	0
1	P	334/336 (99%)	0.02	14 (4%) 36 29	33, 45, 65, 76	0
1	Q	333/336 (99%)	0.44	34 (10%) 6 4	36, 57, 84, 99	0
1	R	334/336 (99%)	0.27	22 (6%) 18 13	33, 50, 72, 85	0
All	All	1335/1344 (99%)	0.21	80 (5%) 21 16	33, 49, 75, 99	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	216	ALA	7.2
1	Q	25	GLU	7.1
1	Q	26	GLY	6.9
1	Q	214	ALA	5.4
1	O	137	GLN	4.9
1	O	62	ASP	4.8
1	P	63	GLY	4.7
1	R	212	GLY	4.4
1	Q	62	ASP	4.3
1	Q	253	ASP	4.3
1	P	335	SER	4.1
1	Q	125	GLY	4.1
1	Q	126	ASP	4.0
1	R	57	GLU	3.9
1	O	212	GLY	3.9
1	R	335	SER	3.7
1	R	261	GLU	3.4
1	Q	60	VAL	3.3
1	R	214	ALA	3.3
1	R	192	ARG	3.3
1	P	104	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	69	GLY	3.2
1	R	334	LEU	3.1
1	R	107	GLN	3.1
1	Q	138	GLU	3.0
1	Q	37	ASP	3.0
1	R	63	GLY	3.0
1	Q	124	THR	2.9
1	Q	303	GLY	2.9
1	P	126	ASP	2.9
1	Q	2	ALA	2.9
1	O	138	GLU	2.8
1	P	265	ASN	2.8
1	Q	31	ALA	2.8
1	Q	304	ASP	2.7
1	P	2	ALA	2.7
1	Q	92	VAL	2.7
1	P	55	THR	2.7
1	R	61	VAL	2.6
1	Q	145	VAL	2.6
1	Q	257	GLU	2.5
1	P	76	SER	2.5
1	O	2	ALA	2.5
1	P	192	ARG	2.5
1	Q	144	THR	2.5
1	R	126	ASP	2.5
1	Q	38	ASP	2.5
1	R	257	GLU	2.4
1	R	62	ASP	2.4
1	Q	114	ALA	2.4
1	P	304	ASP	2.4
1	Q	137	GLN	2.4
1	R	215	LYS	2.4
1	Q	330	TYR	2.4
1	Q	302	VAL	2.4
1	P	253	ASP	2.4
1	O	59	GLU	2.4
1	Q	334	LEU	2.3
1	R	258	GLN	2.3
1	Q	331	LEU	2.3
1	P	334	LEU	2.3
1	R	140	ASP	2.3
1	P	124	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	211	THR	2.3
1	R	38	ASP	2.3
1	Q	116	LYS	2.2
1	Q	123	ALA	2.2
1	Q	24	VAL	2.2
1	R	304	ASP	2.2
1	R	253	ASP	2.1
1	Q	86	LYS	2.1
1	O	214	ALA	2.1
1	Q	88	LEU	2.1
1	R	89	ASN	2.1
1	R	256	VAL	2.1
1	Q	61	VAL	2.1
1	Q	3	VAL	2.0
1	Q	84	PRO	2.0
1	O	68	ASN	2.0
1	P	162	VAL	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 monosaccharides 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, 95<sup>th</sup> 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.

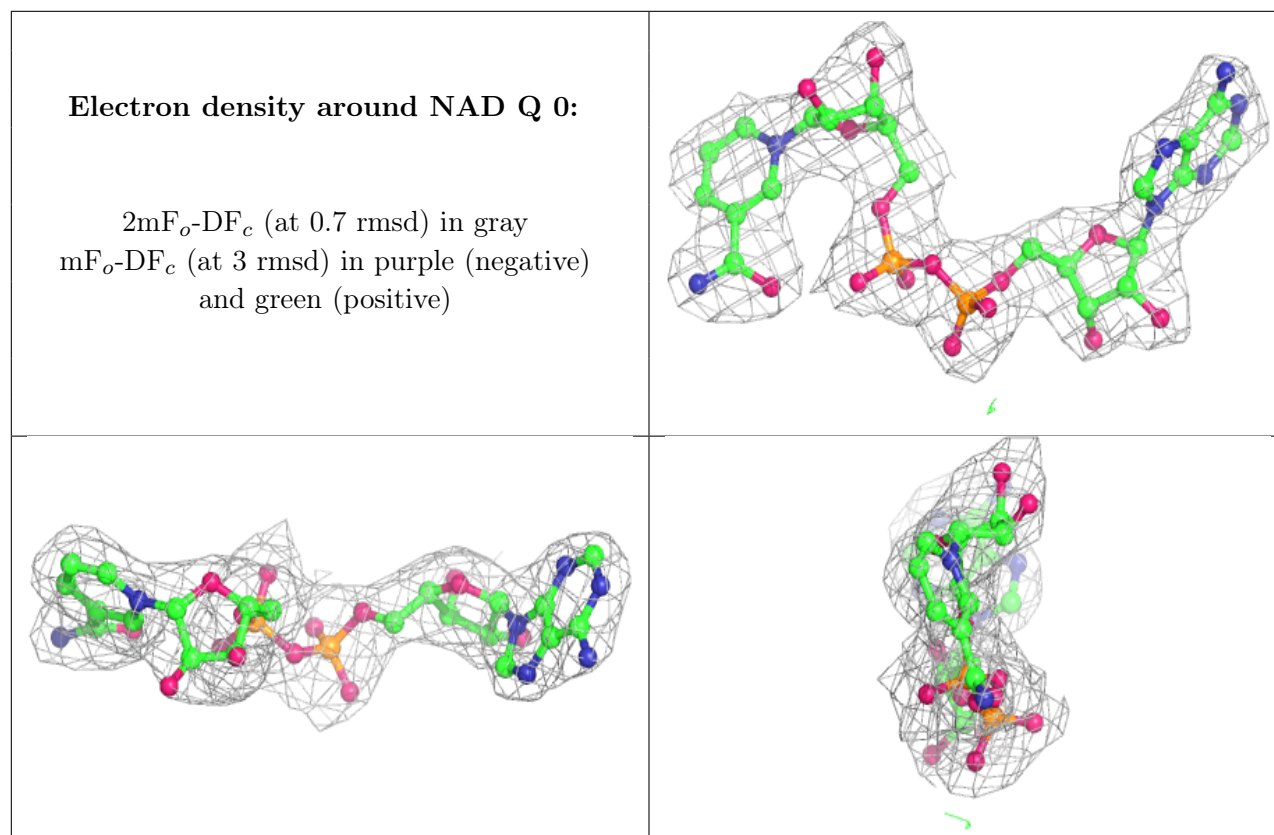
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	3PG	R	337	10/11	0.66	0.38	77,87,91,92	0
3	3PG	O	337	10/11	0.74	0.35	70,78,83,84	0
3	3PG	Q	337	11/11	0.82	0.25	38,58,71,77	0
3	3PG	P	337	11/11	0.85	0.20	45,54,66,68	0
2	NAD	Q	0	44/44	0.95	0.13	27,42,50,55	0
2	NAD	R	0	44/44	0.96	0.12	24,36,41,50	0

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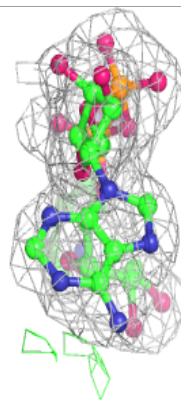
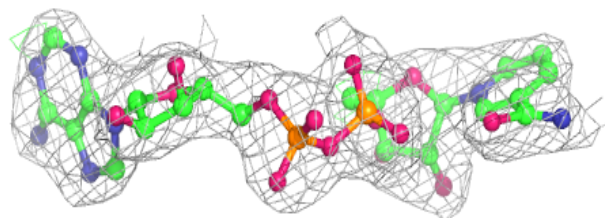
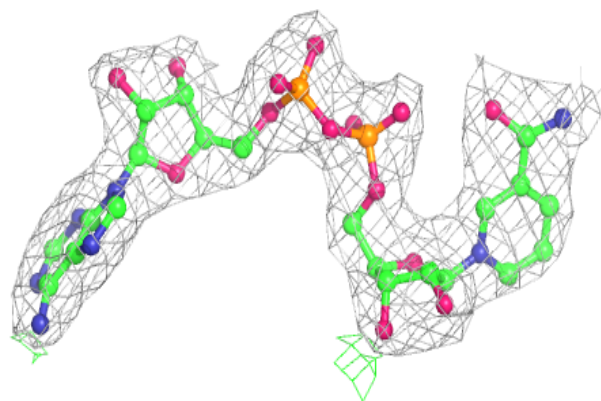
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	O	0	44/44	0.96	0.11	22,34,41,48	0
2	NAD	P	0	44/44	0.98	0.11	18,33,42,45	0

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.

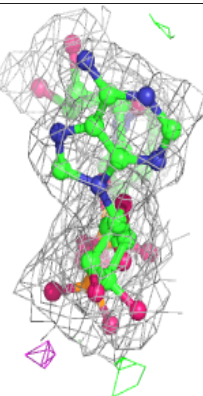
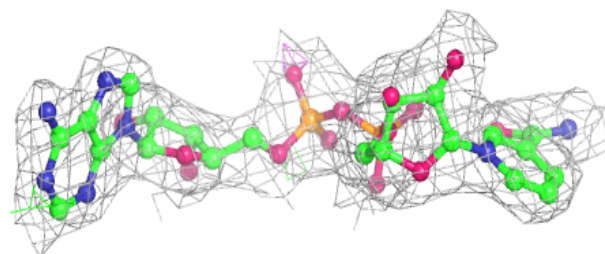
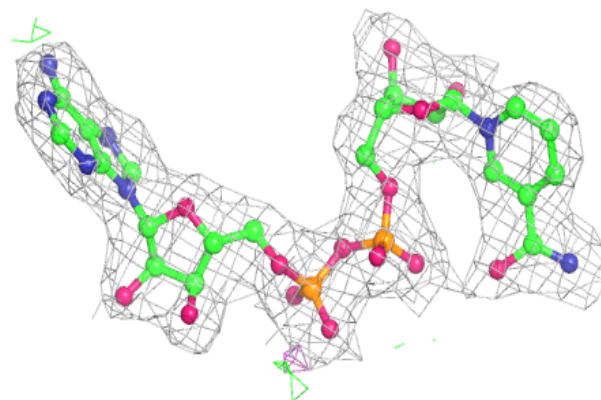


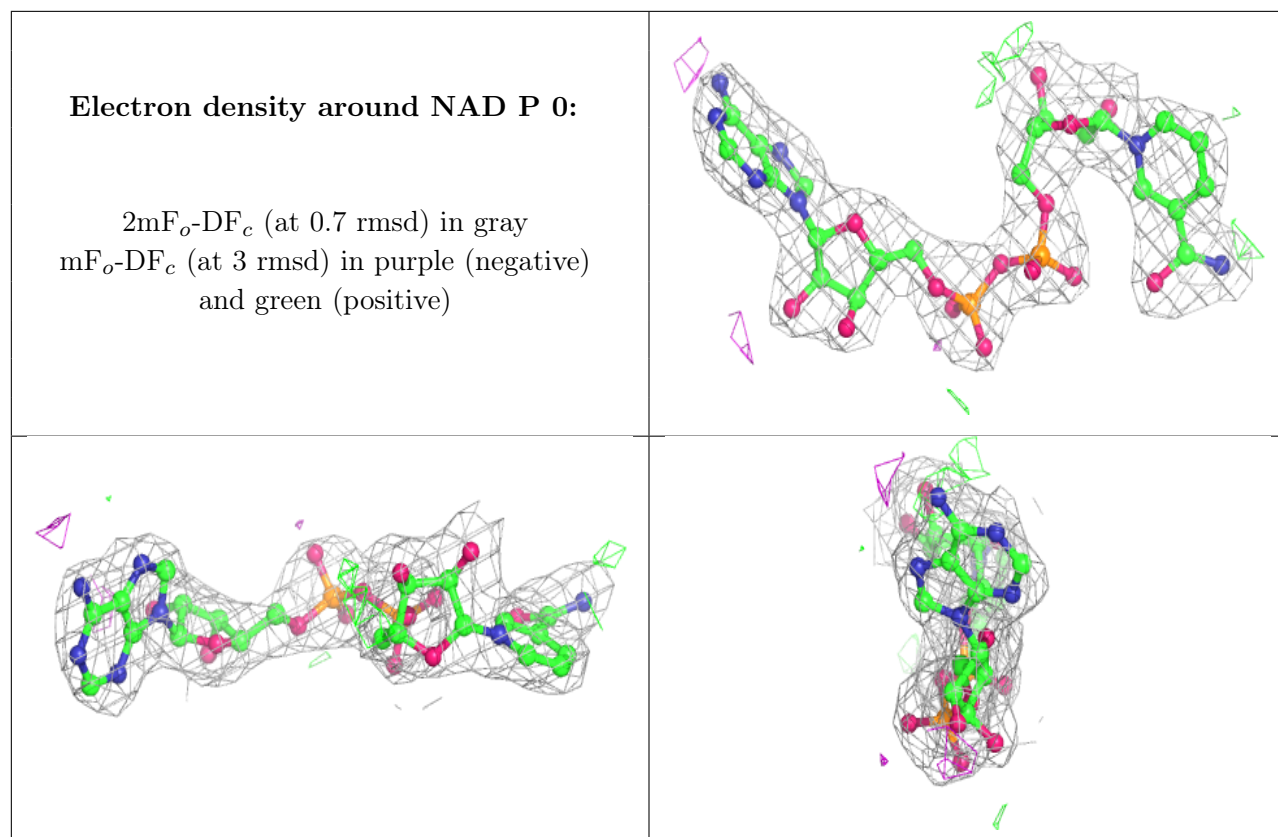
**Electron density around NAD R 0:**

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

**Electron density around NAD O 0:**

$2mF_o-DF_c$  (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.