



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:32 PM EDT

PDB ID : 3B20  
Title : Crystal structure of Glyceraldehyde-3-Phosphate Dehydrogenase complexed with NAD from *Synechococcus elongatus*"  
Authors : Matsumura, H.; Kai, A.; Maeda, T.; Inoue, T.  
Deposited on : 2011-07-17  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

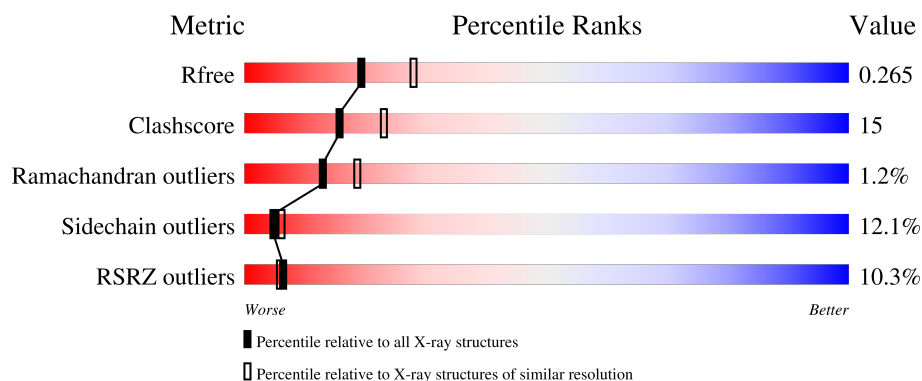
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	339	<div> <div>8%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
1	B	339	<div> <div>%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
1	O	339	<div> <div>2%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	P	339	<div> <div>14%</div> <div>65%</div> <div>30%</div> <div>.</div> </div>
1	Q	339	<div> <div>20%</div> <div>60%</div> <div>33%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	R	339	<div><div></div><div>17%</div><div>60%</div><div>34%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16276 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 (NADP+).

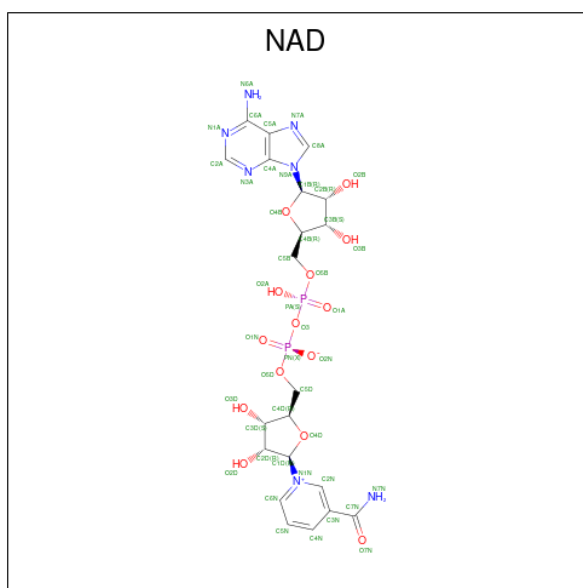
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	B	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	O	337	Total	C	N	O	S	0	0	0
			2588	1628	454	498	8			
1	P	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	Q	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			
1	R	338	Total	C	N	O	S	0	0	0
			2596	1633	455	499	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	O	1	Total 5	O 4	S 1	0	0
2	O	1	Total 5	O 4	S 1	0	0
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	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	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

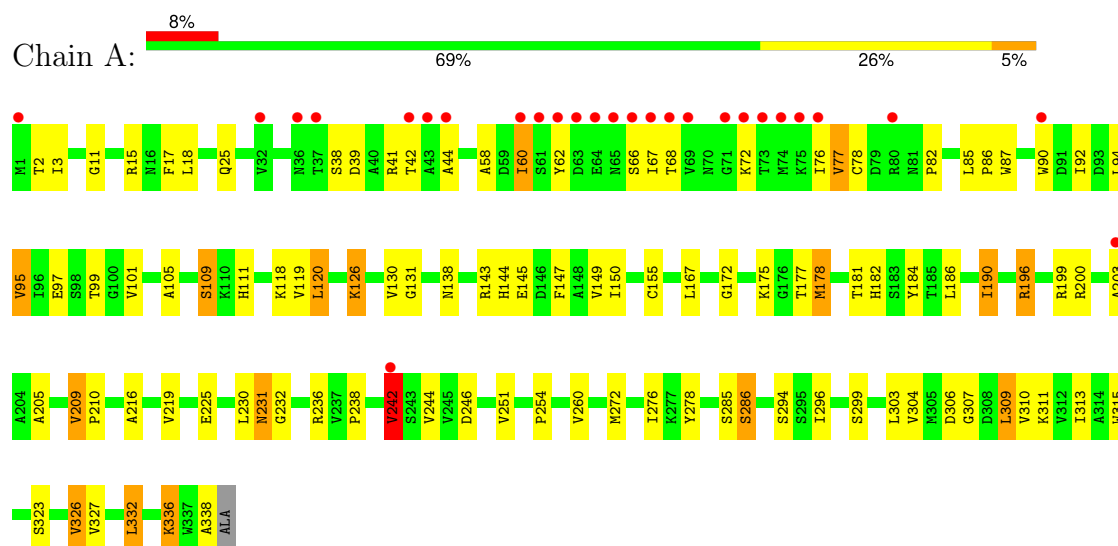
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total 88	O 88	0	0
4	B	106	Total 106	O 106	0	0
4	O	86	Total 86	O 86	0	0
4	P	62	Total 62	O 62	0	0
4	Q	15	Total 15	O 15	0	0
4	R	27	Total 27	O 27	0	0

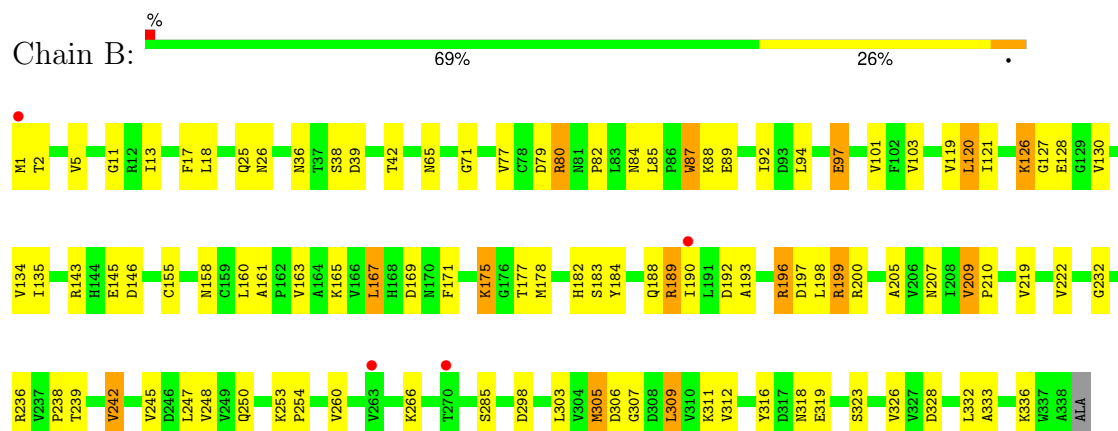
### 3 Residue-property plots [i](#)

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

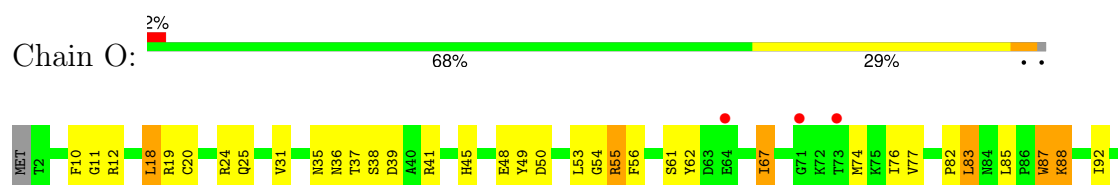
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)

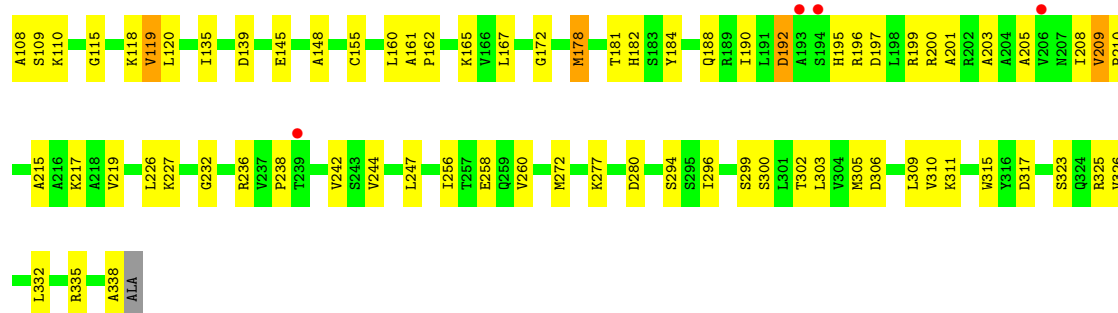


- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)



- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)

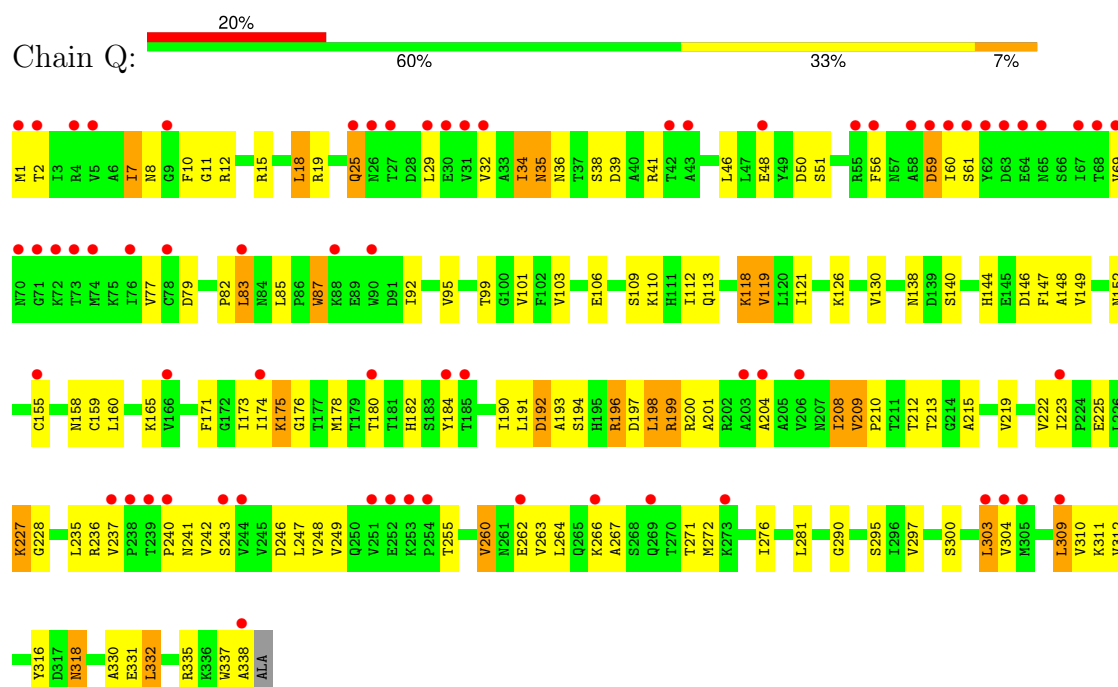




• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)

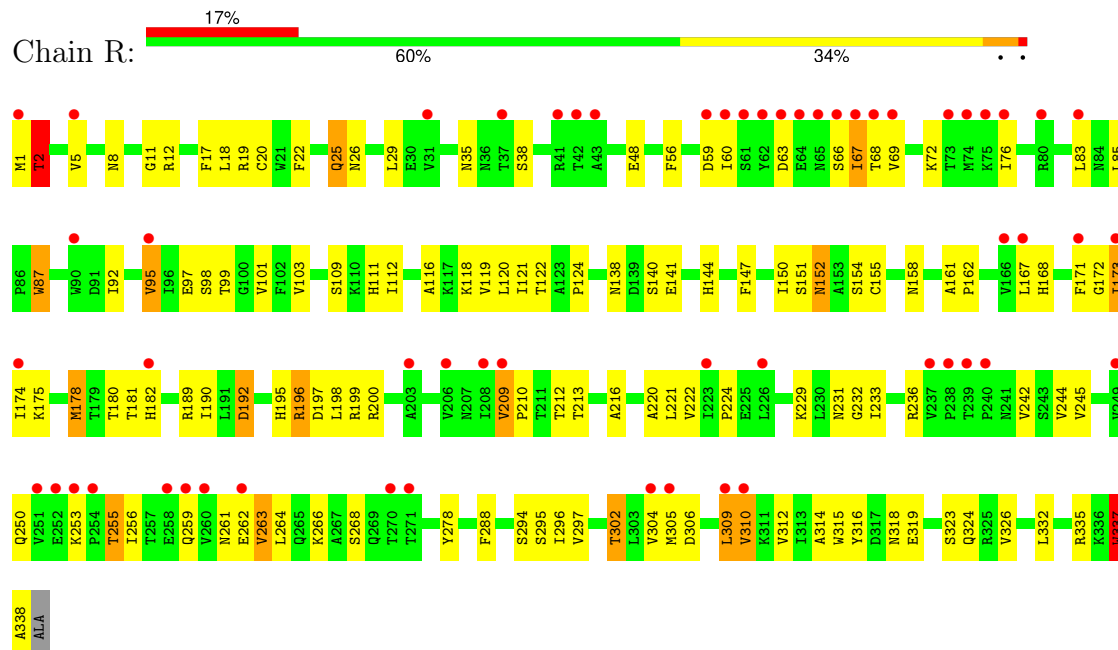


• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)





● Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase (NADP+)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.59Å 79.85Å 206.79Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	45.43 – 2.40 46.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.43-2.40) 99.6 (46.48-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.213 , 0.269 0.211 , 0.265	Depositor DCC
$R_{free}$ test set	4729 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/2639	0.63	0/3590
1	B	0.52	0/2639	0.65	1/3590 (0.0%)
1	O	0.47	0/2631	0.62	0/3580
1	P	0.47	0/2639	0.58	0/3590
1	Q	0.37	0/2639	0.54	0/3590
1	R	0.40	1/2639 (0.0%)	0.54	0/3590
All	All	0.46	1/15826 (0.0%)	0.59	1/21530 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	337	TRP	CB-CG	5.26	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	35	ASN	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2596	0	2620	80	0
1	B	2596	0	2620	84	1
1	O	2588	0	2608	70	0
1	P	2596	0	2620	90	0
1	Q	2596	0	2620	82	0
1	R	2596	0	2620	89	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	O	10	0	0	1	0
2	P	10	0	0	0	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	A	44	0	26	7	0
3	B	44	0	26	5	0
3	O	44	0	26	4	0
3	P	44	0	26	4	0
3	Q	44	0	26	2	0
3	R	44	0	26	5	0
4	A	88	0	0	7	1
4	B	106	0	0	12	0
4	O	86	0	0	6	0
4	P	62	0	0	9	0
4	Q	15	0	0	4	0
4	R	27	0	0	4	0
All	All	16276	0	15864	466	1

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 15.

All (466) 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:A:219:VAL:HG21	1:A:230:LEU:HD12	1.35	1.06
1:A:44:ALA:HB1	1:A:60:ILE:HD11	1.42	1.02
1:B:189:ARG:HG2	1:B:193:ALA:HB3	1.44	0.99
1:B:25:GLN:HG2	1:B:26:ASN:H	1.28	0.96
1:P:144:HIS:HD2	1:P:337:TRP:HA	1.33	0.93
1:A:11:GLY:HA3	3:A:340:NAD:H52A	1.50	0.91
1:R:11:GLY:HA3	3:R:340:NAD:H52A	1.53	0.90
1:O:338:ALA:O	4:O:355:HOH:O	1.90	0.90
1:P:182:HIS:HB3	1:P:236:ARG:HD3	1.57	0.86
1:R:68:THR:O	4:R:358:HOH:O	1.95	0.85
1:B:189:ARG:HH22	1:B:196:ARG:HH22	1.25	0.84
1:P:199:ARG:HD2	1:P:210:PRO:HG2	1.59	0.84
1:A:209:VAL:HG22	1:A:236:ARG:HB2	1.60	0.83
1:O:11:GLY:HA3	3:O:340:NAD:H52A	1.58	0.83
1:R:209:VAL:HG13	1:R:236:ARG:HB2	1.61	0.83
1:B:190:ILE:H	1:B:190:ILE:HD12	1.43	0.82
1:P:128:GLU:O	4:P:376:HOH:O	1.97	0.80
1:P:18:LEU:HD22	1:P:22:PHE:CE1	2.16	0.80
1:A:219:VAL:CG2	1:A:230:LEU:HD12	2.11	0.79
1:P:155:CYS:HB3	3:P:340:NAD:H4N	1.64	0.79
1:Q:118:LYS:HD2	1:Q:148:ALA:HA	1.66	0.78
1:B:222:VAL:O	4:B:393:HOH:O	2.02	0.77
1:R:85:LEU:HD13	1:R:87:TRP:CZ2	2.18	0.77
1:B:333:ALA:O	4:B:343:HOH:O	2.03	0.76
1:P:182:HIS:HB3	1:P:236:ARG:CD	2.17	0.75
1:A:219:VAL:HG21	1:A:230:LEU:CD1	2.16	0.74
1:B:97:GLU:OE2	4:B:420:HOH:O	2.05	0.74
1:P:196:ARG:NH2	4:P:377:HOH:O	2.20	0.74
1:O:197:ASP:HB3	1:O:200:ARG:HB2	1.69	0.74
1:Q:19:ARG:CZ	1:Q:56:PHE:HB2	2.18	0.73
1:A:82:PRO:HA	1:A:85:LEU:HD12	1.70	0.73
1:Q:8:ASN:OD1	1:Q:35:ASN:HB3	1.89	0.73
1:Q:290:GLY:O	4:Q:346:HOH:O	2.06	0.73
1:Q:197:ASP:HB3	1:Q:200:ARG:HB2	1.70	0.73
1:P:246:ASP:OD1	4:P:380:HOH:O	2.07	0.72
1:O:305:MET:HE2	1:P:175:LYS:HB2	1.71	0.72
1:Q:160:LEU:HD11	1:Q:247:LEU:HD13	1.71	0.71
1:R:118:LYS:HE3	1:R:147:PHE:O	1.91	0.71
1:A:105:ALA:O	1:A:109:SER:HB2	1.91	0.71
1:B:196:ARG:CD	1:B:196:ARG:H	2.04	0.71
1:R:168:HIS:HA	1:R:173:ILE:HD13	1.71	0.71
1:B:197:ASP:HB3	1:B:200:ARG:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:144:HIS:CD2	1:P:338:ALA:H	2.09	0.69
1:O:67:ILE:HD12	1:O:76:ILE:HD11	1.74	0.69
1:B:303:LEU:HD12	1:B:311:LYS:HD2	1.75	0.69
1:Q:196:ARG:NE	1:Q:196:ARG:H	1.91	0.69
1:A:216:ALA:O	1:A:219:VAL:HG22	1.91	0.69
1:B:128:GLU:O	4:B:354:HOH:O	2.09	0.69
1:B:71:GLY:N	4:B:397:HOH:O	1.97	0.69
1:O:10:PHE:HZ	1:O:18:LEU:HD12	1.57	0.69
3:P:340:NAD:O3D	4:P:382:HOH:O	2.06	0.68
1:O:303:LEU:HD12	1:O:311:LYS:HD3	1.74	0.68
1:O:256:ILE:HG13	1:O:258:GLU:HG2	1.76	0.68
1:P:44:ALA:O	1:P:60:ILE:HD11	1.93	0.67
1:R:264:LEU:HD13	1:R:297:VAL:HG11	1.75	0.67
1:A:306:ASP:HB3	1:B:175:LYS:HE3	1.77	0.67
1:A:306:ASP:OD1	4:A:386:HOH:O	2.12	0.66
1:R:171:PHE:HE1	1:R:255:THR:HG21	1.60	0.66
1:R:174:ILE:HD12	1:R:250:GLN:HG2	1.78	0.66
1:R:155:CYS:HB3	3:R:340:NAD:H4N	1.77	0.66
1:A:200:ARG:HH12	1:A:236:ARG:NH2	1.93	0.66
1:A:332:LEU:HD22	1:A:336:LYS:HG3	1.76	0.66
1:R:337:TRP:CD1	1:R:337:TRP:C	2.68	0.66
1:B:319:GLU:OE2	4:B:412:HOH:O	2.13	0.65
1:B:163:VAL:HG11	1:B:312:VAL:HG21	1.79	0.65
1:O:182:HIS:HB3	1:O:236:ARG:HD3	1.78	0.65
1:Q:103:VAL:HA	1:Q:121:ILE:HD13	1.78	0.65
1:A:99:THR:OG1	1:A:101:VAL:HG12	1.97	0.64
1:R:337:TRP:CD1	1:R:338:ALA:O	2.50	0.64
1:A:44:ALA:CB	1:A:60:ILE:HD11	2.24	0.64
1:A:119:VAL:CG1	1:A:149:VAL:HG22	2.28	0.64
1:B:25:GLN:HG2	1:B:26:ASN:N	2.08	0.64
1:P:144:HIS:CD2	1:P:337:TRP:HA	2.25	0.64
1:B:199:ARG:NH1	1:B:210:PRO:HG2	2.13	0.64
1:O:209:VAL:HG13	1:O:236:ARG:HB2	1.78	0.64
1:P:186:LEU:HG	1:Q:191:LEU:HB2	1.78	0.64
1:R:197:ASP:HB3	1:R:200:ARG:HB2	1.80	0.64
1:A:119:VAL:HG13	1:A:149:VAL:HG22	1.80	0.63
1:Q:83:LEU:HD13	1:Q:110:LYS:HB3	1.79	0.63
1:A:120:LEU:C	1:A:120:LEU:HD12	2.18	0.63
1:B:205:ALA:HA	1:B:238:PRO:HB3	1.81	0.63
1:Q:182:HIS:HB3	1:Q:236:ARG:HD3	1.81	0.62
1:A:196:ARG:H	1:A:196:ARG:NE	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLU:HB2	4:B:420:HOH:O	2.00	0.62
1:O:10:PHE:CZ	1:O:18:LEU:HD12	2.35	0.61
1:A:311:LYS:NZ	4:A:371:HOH:O	2.32	0.61
1:P:108:ALA:HB1	1:P:119:VAL:HG21	1.82	0.61
1:O:160:LEU:HD23	1:O:219:VAL:CG2	2.31	0.61
1:P:138:ASN:ND2	1:P:222:VAL:HG12	2.15	0.61
1:B:184:TYR:HA	1:B:188:GLN:OE1	2.00	0.61
1:O:323:SER:HA	1:O:326:VAL:HG13	1.83	0.61
1:R:337:TRP:HD1	1:R:338:ALA:O	1.84	0.61
1:A:178:MET:CE	1:A:232:GLY:HA3	2.31	0.61
1:P:17:PHE:HD2	1:P:326:VAL:HG23	1.66	0.61
1:O:45:HIS:CD2	1:R:198:LEU:HG	2.36	0.60
1:B:17:PHE:HD2	1:B:326:VAL:HG22	1.65	0.60
1:O:192:ASP:HB2	1:R:12:ARG:NH1	2.15	0.60
1:P:159:CYS:C	4:P:383:HOH:O	2.39	0.60
1:Q:175:LYS:HE2	1:R:306:ASP:HB3	1.83	0.60
1:B:189:ARG:NH2	1:B:196:ARG:HH22	1.95	0.60
1:P:158:ASN:ND2	4:P:381:HOH:O	2.33	0.60
1:Q:144:HIS:ND1	1:Q:337:TRP:HA	2.16	0.60
1:A:94:LEU:HD12	1:A:118:LYS:O	2.02	0.60
1:B:242:VAL:CG2	1:B:285:SER:HB2	2.32	0.59
1:O:205:ALA:HA	1:O:238:PRO:HB3	1.82	0.59
1:A:323:SER:HA	1:A:326:VAL:HG13	1.85	0.59
1:P:160:LEU:N	4:P:383:HOH:O	2.35	0.59
1:A:155:CYS:H	3:A:340:NAD:H5N	1.68	0.59
1:Q:246:ASP:OD2	1:Q:311:LYS:HE3	2.02	0.59
1:Q:50:ASP:OD2	4:Q:352:HOH:O	2.16	0.59
1:A:231:ASN:OD1	1:B:305:MET:HG2	2.02	0.59
1:P:99:THR:OG1	1:P:101:VAL:HG12	2.02	0.59
1:P:188:GLN:NE2	1:P:209:VAL:HG11	2.18	0.59
1:Q:99:THR:OG1	1:Q:101:VAL:HG12	2.02	0.58
1:O:195:HIS:HB3	1:O:201:ALA:HB2	1.86	0.58
1:B:82:PRO:HA	1:B:85:LEU:HD12	1.85	0.58
1:O:48:GLU:O	1:O:55:ARG:HA	2.03	0.58
1:P:12:ARG:HH11	1:Q:192:ASP:HB2	1.67	0.58
1:P:198:LEU:HD12	1:P:198:LEU:H	1.69	0.58
1:R:120:LEU:HD13	1:R:150:ILE:HG13	1.84	0.58
1:R:161:ALA:HB3	1:R:162:PRO:HD3	1.86	0.58
1:P:120:LEU:HD13	1:P:150:ILE:HG13	1.85	0.58
1:Q:152:ASN:ND2	4:Q:345:HOH:O	2.33	0.57
1:O:192:ASP:HB2	1:R:12:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:260:VAL:HG22	1:O:302:THR:HG21	1.87	0.57
1:A:155:CYS:HB3	3:A:340:NAD:H4N	1.86	0.57
1:O:36:ASN:HB3	4:O:371:HOH:O	2.05	0.57
1:B:182:HIS:HB3	1:B:236:ARG:HD3	1.85	0.57
1:P:209:VAL:HG13	1:P:236:ARG:HB2	1.86	0.57
1:R:25:GLN:CD	1:R:25:GLN:H	2.08	0.57
1:Q:176:GLY:HA3	1:Q:249:VAL:HG12	1.87	0.56
1:B:196:ARG:H	1:B:196:ARG:NE	2.03	0.56
1:P:12:ARG:NH1	1:Q:192:ASP:HB2	2.20	0.56
1:B:155:CYS:HB3	3:B:340:NAD:H4N	1.88	0.56
1:A:182:HIS:HB3	1:A:236:ARG:HD3	1.88	0.56
1:Q:87:TRP:HA	1:Q:87:TRP:CE3	2.41	0.56
1:P:87:TRP:CE3	1:P:92:ILE:HG13	2.40	0.56
1:A:11:GLY:O	1:A:15:ARG:HG3	2.06	0.56
1:R:167:LEU:HB3	1:R:173:ILE:HD11	1.88	0.55
4:A:371:HOH:O	1:B:177:THR:HG23	2.06	0.55
1:Q:29:LEU:HD21	1:Q:330:ALA:O	2.06	0.55
1:P:103:VAL:HA	1:P:121:ILE:HD13	1.88	0.55
1:P:181:THR:HB	1:P:244:VAL:HG12	1.87	0.55
1:Q:171:PHE:CE1	1:Q:255:THR:HB	2.41	0.55
1:O:83:LEU:HD13	1:O:110:LYS:HB3	1.88	0.55
1:Q:175:LYS:HD3	1:R:305:MET:O	2.06	0.55
1:Q:87:TRP:HA	1:Q:87:TRP:HE3	1.71	0.55
1:R:175:LYS:HE3	1:R:250:GLN:HE21	1.73	0.54
1:R:261:ASN:HB3	1:R:278:TYR:OH	2.07	0.54
1:A:242:VAL:CG2	1:A:285:SER:HB2	2.38	0.54
1:O:31:VAL:O	1:O:74:MET:HG2	2.07	0.54
1:R:196:ARG:H	1:R:196:ARG:HE	1.56	0.54
1:A:296:ILE:HB	1:A:315:TRP:HB2	1.90	0.54
1:P:190:ILE:CD1	1:Q:204:ALA:HB3	2.38	0.54
1:A:87:TRP:CE3	1:A:92:ILE:HG13	2.42	0.54
1:P:18:LEU:HD22	1:P:22:PHE:HE1	1.72	0.54
1:A:144:HIS:CG	1:A:338:ALA:H	2.26	0.53
1:O:82:PRO:HA	1:O:85:LEU:HD12	1.89	0.53
1:A:323:SER:O	1:A:327:VAL:HG23	2.08	0.53
1:P:197:ASP:HB3	1:P:200:ARG:HB2	1.90	0.53
1:Q:175:LYS:HD3	1:R:306:ASP:HB3	1.89	0.53
1:Q:196:ARG:H	1:Q:196:ARG:HE	1.55	0.53
1:B:36:ASN:HB3	4:B:349:HOH:O	2.09	0.53
1:O:335:ARG:NH1	4:O:394:HOH:O	2.42	0.53
1:Q:25:GLN:H	1:Q:25:GLN:CD	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:305:MET:HG2	1:P:231:ASN:ND2	2.24	0.53
1:B:25:GLN:CG	1:B:26:ASN:H	2.12	0.53
1:O:208:ILE:HB	1:P:285:SER:HB3	1.90	0.53
1:R:302:THR:HG23	1:R:312:VAL:HG22	1.90	0.52
3:B:340:NAD:O1A	3:B:340:NAD:O1N	2.26	0.52
1:R:99:THR:OG1	1:R:101:VAL:HG22	2.10	0.52
1:R:155:CYS:HB3	3:R:340:NAD:C4N	2.40	0.52
1:O:181:THR:HB	1:O:244:VAL:HG12	1.92	0.52
1:A:315:TRP:HZ2	1:B:210:PRO:HG3	1.74	0.52
1:P:155:CYS:CB	3:P:340:NAD:H4N	2.38	0.52
1:O:182:HIS:HB3	1:O:236:ARG:CD	2.40	0.52
1:O:306:ASP:HB3	1:P:175:LYS:HD3	1.92	0.52
1:P:155:CYS:HB3	3:P:340:NAD:C4N	2.39	0.52
1:A:155:CYS:SG	3:A:340:NAD:H4N	2.50	0.52
1:Q:209:VAL:HG23	1:Q:236:ARG:O	2.10	0.52
1:Q:227:LYS:NZ	1:Q:228:GLY:H	2.08	0.51
1:O:280:ASP:HA	1:O:299:SER:OG	2.10	0.51
1:R:144:HIS:NE2	1:R:338:ALA:HA	2.26	0.51
1:B:323:SER:HA	1:B:326:VAL:HG13	1.93	0.51
1:R:212:THR:HB	4:R:363:HOH:O	2.09	0.51
1:Q:7:ILE:HG13	1:Q:34:ILE:HD13	1.93	0.51
1:P:40:ALA:HB1	1:P:67:ILE:HD12	1.92	0.51
1:P:159:CYS:HA	4:P:383:HOH:O	2.11	0.51
1:R:221:LEU:N	1:R:221:LEU:HD23	2.25	0.51
1:A:184:TYR:CD2	1:A:238:PRO:HA	2.46	0.51
1:O:184:TYR:CD2	1:O:238:PRO:HA	2.45	0.51
1:P:17:PHE:CD2	1:P:326:VAL:HG23	2.46	0.51
1:R:112:ILE:HA	1:R:116:ALA:O	2.11	0.51
1:A:286:SER:HB3	1:B:207:ASN:OD1	2.11	0.51
1:A:143:ARG:NH1	4:A:385:HOH:O	2.39	0.50
1:A:175:LYS:HD3	1:B:306:ASP:HB3	1.93	0.50
1:O:165:LYS:HD3	1:O:272:MET:CE	2.40	0.50
1:R:1:MET:O	1:R:2:THR:HB	2.10	0.50
1:B:245:VAL:HG23	1:B:316:TYR:CE1	2.46	0.50
1:Q:119:VAL:HG13	1:Q:149:VAL:HG22	1.94	0.50
1:R:19:ARG:CZ	1:R:56:PHE:HB2	2.42	0.50
1:R:216:ALA:CB	1:R:231:ASN:HA	2.42	0.50
1:B:189:ARG:NH2	1:B:196:ARG:NH2	2.60	0.50
1:R:175:LYS:HE3	1:R:250:GLN:NE2	2.27	0.50
1:A:144:HIS:HD2	4:A:354:HOH:O	1.94	0.50
1:Q:159:CYS:HG	1:Q:316:TYR:HD1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD13	1:A:150:ILE:HG13	1.93	0.50
1:A:309:LEU:HB2	1:B:175:LYS:HD2	1.93	0.50
1:O:87:TRP:HA	1:O:87:TRP:CE3	2.47	0.50
1:O:215:ALA:HB2	2:O:3339:SO4:O2	2.11	0.50
1:P:199:ARG:CD	1:P:210:PRO:HG2	2.35	0.50
1:O:205:ALA:HB3	4:O:360:HOH:O	2.11	0.49
1:Q:337:TRP:CD1	1:Q:338:ALA:N	2.79	0.49
1:A:2:THR:HG22	1:A:3:ILE:N	2.27	0.49
1:P:95:VAL:HG13	1:P:119:VAL:HB	1.95	0.49
1:R:85:LEU:HD13	1:R:87:TRP:CE2	2.48	0.49
1:P:87:TRP:CE3	1:P:87:TRP:HA	2.47	0.49
1:P:190:ILE:HD11	1:Q:204:ALA:HB3	1.93	0.49
1:Q:106:GLU:O	1:Q:109:SER:HB2	2.11	0.49
1:P:35:ASN:HA	1:P:77:VAL:HG13	1.93	0.49
1:P:87:TRP:HA	1:P:87:TRP:HE3	1.77	0.49
1:P:160:LEU:HD12	1:P:160:LEU:O	2.12	0.49
1:P:260:VAL:HG23	1:P:302:THR:HG21	1.94	0.49
1:B:199:ARG:HH11	1:B:210:PRO:HG2	1.77	0.49
1:Q:48:GLU:HB2	1:Q:60:ILE:HD12	1.95	0.49
1:P:19:ARG:NH2	1:P:50:ASP:HB2	2.28	0.49
1:A:225:GLU:HB2	4:A:412:HOH:O	2.11	0.49
1:B:143:ARG:HB2	1:B:146:ASP:OD1	2.13	0.49
1:A:86:PRO:HG2	1:A:90:TRP:CE3	2.47	0.48
1:A:205:ALA:HA	1:A:238:PRO:HB3	1.94	0.48
1:B:80:ARG:CG	1:B:80:ARG:HH11	2.26	0.48
3:O:340:NAD:H51A	4:O:413:HOH:O	2.12	0.48
1:Q:11:GLY:O	1:Q:15:ARG:HG3	2.13	0.48
1:R:189:ARG:CZ	1:R:195:HIS:HD2	2.26	0.48
1:O:260:VAL:CG2	1:O:302:THR:HG21	2.43	0.48
1:P:8:ASN:OD1	1:P:35:ASN:HB3	2.14	0.48
1:A:41:ARG:HG3	1:A:62:TYR:OH	2.13	0.48
1:A:177:THR:CB	1:A:231:ASN:HD21	2.26	0.48
1:O:20:CYS:O	1:O:24:ARG:HG2	2.12	0.48
1:P:118:LYS:NZ	1:P:147:PHE:O	2.47	0.48
1:R:22:PHE:CZ	1:R:69:VAL:HB	2.48	0.48
1:B:190:ILE:H	1:B:190:ILE:CD1	2.17	0.48
1:R:168:HIS:CA	1:R:173:ILE:HD13	2.43	0.48
1:P:76:ILE:HG22	1:P:77:VAL:N	2.29	0.48
1:A:254:PRO:HA	1:A:307:GLY:O	2.14	0.48
1:O:87:TRP:HA	1:O:87:TRP:HE3	1.78	0.48
1:P:196:ARG:H	1:P:196:ARG:NE	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASN:HD22	1:A:231:ASN:H	1.62	0.48
1:O:12:ARG:NH1	1:R:192:ASP:HB2	2.28	0.48
1:R:337:TRP:C	1:R:337:TRP:HD1	2.15	0.48
1:Q:112:ILE:HD11	1:Q:119:VAL:HG12	1.95	0.48
1:P:159:CYS:O	1:P:159:CYS:SG	2.72	0.48
1:Q:165:LYS:HB2	1:Q:223:ILE:HD11	1.96	0.48
1:A:118:LYS:HE3	1:A:144:HIS:CD2	2.49	0.47
1:Q:173:ILE:HG23	1:Q:249:VAL:HB	1.95	0.47
1:B:247:LEU:O	1:B:311:LYS:HA	2.14	0.47
1:B:87:TRP:CE3	1:B:92:ILE:HG13	2.49	0.47
1:B:145:GLU:OE1	1:B:145:GLU:N	2.42	0.47
1:R:95:VAL:HG13	1:R:119:VAL:HB	1.97	0.47
1:R:178:MET:O	1:R:232:GLY:HA3	2.14	0.47
1:B:160:LEU:HD11	1:B:247:LEU:HD13	1.96	0.47
1:P:161:ALA:HB3	1:P:162:PRO:HD3	1.96	0.47
1:R:17:PHE:HD2	1:R:326:VAL:HG22	1.80	0.47
1:R:48:GLU:HA	1:R:56:PHE:HB3	1.97	0.47
1:R:87:TRP:HA	1:R:87:TRP:HE3	1.80	0.47
1:R:92:ILE:O	1:R:116:ALA:HA	2.14	0.47
1:A:199:ARG:NH2	1:B:298:ASP:OD1	2.48	0.47
1:B:158:ASN:ND2	4:B:345:HOH:O	2.41	0.47
1:P:159:CYS:CA	4:P:383:HOH:O	2.63	0.47
1:Q:303:LEU:HD22	1:Q:304:VAL:H	1.80	0.47
1:B:178:MET:O	1:B:232:GLY:HA2	2.15	0.46
1:R:335:ARG:NH1	4:R:352:HOH:O	2.47	0.46
1:P:277:LYS:HB3	1:P:296:ILE:HG23	1.98	0.46
1:Q:248:VAL:HG22	1:Q:311:LYS:HG3	1.98	0.46
1:O:145:GLU:CD	1:O:145:GLU:H	2.18	0.46
1:O:190:ILE:HA	1:R:190:ILE:HD12	1.97	0.46
1:O:199:ARG:CZ	1:P:282:PRO:HA	2.46	0.46
1:P:18:LEU:CD2	1:P:22:PHE:CE1	2.92	0.46
1:R:20:CYS:HB3	1:R:324:GLN:OE1	2.16	0.46
1:O:178:MET:O	1:O:232:GLY:HA2	2.16	0.46
1:A:190:ILE:H	1:A:190:ILE:HG13	1.55	0.46
1:O:209:VAL:HA	1:O:210:PRO:HD3	1.86	0.46
1:R:181:THR:HB	1:R:244:VAL:HG12	1.98	0.46
1:A:278:TYR:CE1	1:A:299:SER:HB3	2.50	0.46
1:O:155:CYS:SG	3:O:340:NAD:C4N	3.04	0.46
1:R:11:GLY:HA3	3:R:340:NAD:O1A	2.15	0.46
1:B:196:ARG:H	1:B:196:ARG:HD2	1.80	0.46
1:R:59:ASP:O	1:R:69:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:SG	3:A:340:NAD:C4N	3.05	0.45
1:A:304:VAL:HG22	1:A:310:VAL:HB	1.98	0.45
1:A:17:PHE:HD2	1:A:326:VAL:HG22	1.80	0.45
1:P:206:VAL:HG11	1:Q:240:PRO:HG3	1.98	0.45
1:R:245:VAL:HG13	1:R:316:TYR:CE1	2.51	0.45
1:B:209:VAL:HA	1:B:210:PRO:HD3	1.72	0.45
1:O:108:ALA:HB1	1:O:119:VAL:HG21	1.99	0.45
1:A:67:ILE:HG12	1:A:76:ILE:HD11	1.98	0.45
1:P:22:PHE:HZ	1:P:74:MET:CE	2.29	0.45
1:P:184:TYR:CE2	1:P:238:PRO:HA	2.51	0.45
1:Q:182:HIS:HA	1:Q:243:SER:HB3	1.99	0.45
1:A:242:VAL:HG22	1:A:285:SER:HB2	1.98	0.45
1:O:160:LEU:HD23	1:O:219:VAL:HG21	1.98	0.45
1:O:247:LEU:O	1:O:311:LYS:HA	2.17	0.45
1:P:48:GLU:HG2	1:P:49:TYR:CE2	2.51	0.45
1:B:165:LYS:HD3	1:B:169:ASP:OD2	2.16	0.45
1:R:304:VAL:HG22	1:R:310:VAL:HG13	1.98	0.45
1:B:89:GLU:H	1:B:89:GLU:CD	2.20	0.45
1:P:50:ASP:OD2	1:P:53:LEU:HD12	2.17	0.45
1:Q:146:ASP:HB3	1:Q:147:PHE:CD1	2.52	0.45
1:R:5:VAL:HG21	1:R:29:LEU:HD22	1.99	0.45
1:R:87:TRP:HA	1:R:87:TRP:CE3	2.52	0.45
1:R:152:ASN:OD1	1:R:326:VAL:HA	2.17	0.45
1:P:17:PHE:HD2	1:P:326:VAL:CG2	2.27	0.45
1:Q:29:LEU:HG	1:Q:331:GLU:OE1	2.15	0.45
1:A:181:THR:HB	1:A:244:VAL:HG12	1.99	0.45
1:R:305:MET:HB2	1:R:309:LEU:HB3	1.99	0.45
1:A:178:MET:HE2	1:A:178:MET:HB3	1.57	0.44
1:Q:182:HIS:HB3	1:Q:236:ARG:CD	2.47	0.44
1:R:199:ARG:HD2	1:R:210:PRO:HD2	1.99	0.44
1:A:11:GLY:HA3	3:A:340:NAD:O2A	2.16	0.44
1:Q:25:GLN:CD	1:Q:25:GLN:N	2.70	0.44
1:B:17:PHE:CD2	1:B:326:VAL:HG22	2.49	0.44
1:B:183:SER:HB3	1:B:239:THR:O	2.17	0.44
1:B:236:ARG:NE	4:B:403:HOH:O	2.16	0.44
1:O:217:LYS:NZ	4:O:380:HOH:O	2.51	0.44
1:P:85:LEU:HD13	1:P:87:TRP:CZ2	2.52	0.44
1:P:45:HIS:ND1	1:Q:198:LEU:HG	2.33	0.44
1:P:202:ARG:HH21	1:Q:51:SER:N	2.15	0.44
1:Q:264:LEU:HD13	1:Q:297:VAL:HG11	1.99	0.44
1:R:95:VAL:HG11	1:R:111:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ASP:HB3	4:B:434:HOH:O	2.17	0.44
1:P:200:ARG:HH22	1:P:236:ARG:NH2	2.15	0.44
1:A:95:VAL:HG11	1:A:111:HIS:HB3	2.00	0.44
1:O:87:TRP:CE3	1:O:92:ILE:HG13	2.53	0.44
1:A:231:ASN:CG	1:B:305:MET:HG2	2.38	0.44
1:B:163:VAL:CG1	1:B:312:VAL:HG21	2.46	0.44
1:Q:83:LEU:HD12	1:Q:83:LEU:HA	1.90	0.44
1:Q:87:TRP:CE3	1:Q:92:ILE:HG13	2.52	0.44
1:R:323:SER:HA	1:R:326:VAL:HG13	1.99	0.44
1:A:17:PHE:CD2	1:A:326:VAL:HG22	2.52	0.44
1:A:246:ASP:HA	1:A:313:ILE:HD13	2.00	0.44
1:B:184:TYR:CD2	1:B:238:PRO:HA	2.53	0.44
1:P:198:LEU:HD12	1:P:198:LEU:N	2.33	0.44
1:Q:267:ALA:O	1:Q:272:MET:N	2.46	0.44
1:R:98:SER:HA	1:R:122:THR:OG1	2.18	0.44
1:R:198:LEU:HA	1:R:198:LEU:HD12	1.75	0.44
1:B:189:ARG:HH22	1:B:196:ARG:NH2	2.03	0.43
1:R:66:SER:HA	1:R:76:ILE:HG12	1.99	0.43
1:R:182:HIS:HB3	1:R:236:ARG:HE	1.83	0.43
1:P:278:TYR:CE1	1:P:299:SER:HB3	2.52	0.43
1:R:245:VAL:HG13	1:R:316:TYR:HE1	1.84	0.43
1:A:126:LYS:HD2	4:A:343:HOH:O	2.17	0.43
1:Q:35:ASN:OD1	1:Q:77:VAL:HG13	2.18	0.43
1:Q:82:PRO:HA	1:Q:85:LEU:HD12	2.01	0.43
1:Q:193:ALA:O	1:Q:201:ALA:HB1	2.18	0.43
1:O:226:LEU:HD23	1:O:226:LEU:HA	1.75	0.43
1:O:296:ILE:HB	1:O:315:TRP:HB2	2.00	0.43
1:P:220:ALA:HB2	1:P:227:LYS:HA	2.01	0.43
1:Q:59:ASP:O	1:Q:69:VAL:HA	2.19	0.43
1:A:58:ALA:O	1:A:60:ILE:HG22	2.18	0.43
1:A:272:MET:HG3	1:A:276:ILE:HD12	2.00	0.43
1:P:254:PRO:HA	1:P:307:GLY:O	2.18	0.43
1:A:62:TYR:HB2	1:A:67:ILE:HG22	2.00	0.43
1:A:178:MET:HE2	1:A:232:GLY:HA3	1.99	0.43
1:A:246:ASP:OD2	1:A:311:LYS:HE3	2.17	0.43
1:B:336:LYS:HA	1:B:336:LYS:HD3	1.68	0.43
1:O:41:ARG:HG3	1:O:62:TYR:OH	2.18	0.43
1:Q:332:LEU:HD23	1:Q:332:LEU:HA	1.84	0.43
1:P:48:GLU:HB2	1:P:60:ILE:HD13	2.01	0.43
1:Q:260:VAL:HA	1:Q:263:VAL:HG12	2.01	0.43
1:R:109:SER:HA	1:R:112:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:171:PHE:CE1	1:R:255:THR:HG21	2.46	0.43
1:O:317:ASP:C	1:O:317:ASP:OD1	2.57	0.43
1:Q:184:TYR:HA	1:Q:236:ARG:HD2	2.01	0.43
1:A:77:VAL:HG12	1:A:78:CYS:H	1.84	0.42
1:B:11:GLY:HA3	3:B:340:NAD:O1A	2.19	0.42
1:Q:138:ASN:ND2	1:Q:222:VAL:HG12	2.33	0.42
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.87	0.42
1:P:18:LEU:HD22	1:P:22:PHE:CD1	2.52	0.42
1:O:165:LYS:HD3	1:O:272:MET:HE1	2.02	0.42
1:P:67:ILE:HB	1:P:76:ILE:HD11	2.01	0.42
1:P:82:PRO:HA	1:P:85:LEU:HG	2.00	0.42
1:Q:155:CYS:HB3	3:Q:340:NAD:H4N	2.00	0.42
1:B:5:VAL:HA	1:B:94:LEU:O	2.20	0.42
1:O:49:TYR:OH	1:Q:281:LEU:HD13	2.20	0.42
1:Q:19:ARG:HD3	1:Q:56:PHE:CD1	2.54	0.42
1:B:135:ILE:HG13	1:B:328:ASP:HB3	2.01	0.42
1:O:199:ARG:NH1	1:O:210:PRO:HG2	2.35	0.42
1:Q:159:CYS:SG	1:Q:316:TYR:CD1	3.13	0.42
1:Q:208:ILE:HG23	1:Q:237:VAL:HG12	2.02	0.42
1:Q:227:LYS:HZ1	1:Q:228:GLY:H	1.68	0.42
1:R:8:ASN:OD1	1:R:35:ASN:HB3	2.20	0.42
1:R:103:VAL:HA	1:R:121:ILE:HD13	2.01	0.42
1:R:196:ARG:H	1:R:196:ARG:NE	2.17	0.42
1:R:213:THR:N	4:R:363:HOH:O	2.22	0.42
1:O:35:ASN:HA	1:O:77:VAL:O	2.18	0.42
1:O:199:ARG:HH11	1:O:210:PRO:HG2	1.85	0.42
1:P:260:VAL:HG23	1:P:261:ASN:N	2.34	0.42
1:R:171:PHE:CE2	1:R:263:VAL:HG21	2.54	0.42
1:A:209:VAL:HA	1:A:210:PRO:HD3	1.97	0.42
1:O:155:CYS:SG	3:O:340:NAD:H4N	2.60	0.42
1:P:28:ASP:N	1:P:331:GLU:OE2	2.43	0.42
1:Q:36:ASN:C	1:Q:38:SER:H	2.23	0.42
1:R:182:HIS:HB3	1:R:236:ARG:NE	2.35	0.42
1:P:81:ASN:HA	1:P:82:PRO:HD3	1.87	0.42
1:Q:309:LEU:HB2	1:R:175:LYS:HD2	2.01	0.42
1:R:56:PHE:CD2	1:R:60:ILE:HD11	2.55	0.42
1:R:124:PRO:HG3	1:R:154:SER:HB3	2.02	0.42
1:R:220:ALA:O	1:R:224:PRO:HA	2.20	0.42
1:R:318:ASN:O	3:R:340:NAD:H4N	2.20	0.42
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.82	0.42
1:B:316:TYR:CD1	1:B:316:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:39:ASP:HB2	4:Q:343:HOH:O	2.19	0.42
1:A:68:THR:HG23	1:A:72:LYS:O	2.19	0.42
1:R:12:ARG:NE	1:R:319:GLU:OE2	2.52	0.42
1:R:174:ILE:HG22	1:R:175:LYS:HE2	2.02	0.42
1:B:177:THR:HG22	1:B:248:VAL:HB	2.01	0.41
1:P:188:GLN:HE22	1:P:209:VAL:HG11	1.82	0.41
1:Q:18:LEU:HA	1:Q:18:LEU:HD23	1.61	0.41
1:Q:199:ARG:HD2	1:Q:210:PRO:HG2	2.01	0.41
1:O:135:ILE:HB	1:O:325:ARG:HD3	2.01	0.41
1:P:25:GLN:HB2	1:P:26:ASN:H	1.52	0.41
1:P:29:LEU:HD21	1:P:331:GLU:HA	2.02	0.41
1:B:103:VAL:HA	1:B:121:ILE:HD13	2.02	0.41
1:B:134:VAL:HG11	1:B:161:ALA:HB3	2.02	0.41
1:B:175:LYS:NZ	1:B:250:GLN:OE1	2.51	0.41
1:Q:215:ALA:O	1:Q:219:VAL:HG23	2.20	0.41
1:A:38:SER:OG	1:A:42:THR:HB	2.21	0.41
1:B:13:ILE:HG13	3:B:340:NAD:O4D	2.20	0.41
1:B:38:SER:OG	1:B:42:THR:HB	2.20	0.41
1:O:305:MET:HG3	1:P:176:GLY:O	2.21	0.41
1:Q:255:THR:O	1:Q:304:VAL:HG11	2.20	0.41
1:A:131:GLY:HA3	1:A:147:PHE:CD1	2.55	0.41
1:O:184:TYR:HA	1:O:188:GLN:OE1	2.21	0.41
1:R:174:ILE:O	1:R:229:LYS:HE2	2.20	0.41
1:B:242:VAL:HG22	1:B:285:SER:HB2	2.03	0.41
1:P:220:ALA:O	1:P:224:PRO:HA	2.21	0.41
1:Q:241:ASN:OD1	1:Q:318:ASN:ND2	2.54	0.41
1:A:178:MET:CE	1:A:178:MET:O	2.69	0.41
1:B:199:ARG:HD2	1:B:210:PRO:HD2	2.02	0.41
1:O:118:LYS:HG3	1:O:148:ALA:O	2.20	0.41
1:B:319:GLU:CG	4:B:412:HOH:O	2.68	0.41
1:O:50:ASP:OD2	1:O:53:LEU:HD12	2.20	0.41
1:O:88:LYS:HB2	1:O:115:GLY:HA3	2.03	0.41
1:O:161:ALA:HB3	1:O:162:PRO:HD3	2.01	0.41
1:R:288:PHE:CE1	1:R:315:TRP:CD1	3.09	0.41
1:R:296:ILE:O	1:R:314:ALA:HA	2.21	0.41
1:A:155:CYS:CB	3:A:340:NAD:H4N	2.49	0.41
1:B:245:VAL:HG23	1:B:316:TYR:HE1	1.85	0.41
1:P:120:LEU:C	1:P:120:LEU:HD12	2.41	0.41
1:R:138:ASN:HD21	1:R:222:VAL:HG12	1.86	0.41
1:B:87:TRP:HE3	1:B:87:TRP:HA	1.86	0.40
1:P:92:ILE:O	1:P:116:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:185:THR:HG23	1:P:236:ARG:NH1	2.35	0.40
1:Q:12:ARG:HG2	3:Q:340:NAD:O2A	2.21	0.40
1:Q:309:LEU:HD23	1:Q:309:LEU:HA	1.85	0.40
1:B:126:LYS:HE3	1:B:127:GLY:N	2.36	0.40
1:B:171:PHE:O	1:B:253:LYS:HD2	2.21	0.40
1:B:254:PRO:HA	1:B:307:GLY:O	2.21	0.40
1:B:318:ASN:O	3:B:340:NAD:H4N	2.22	0.40
1:Q:130:VAL:HG13	1:Q:149:VAL:HG12	2.04	0.40
1:Q:235:LEU:HD23	1:Q:235:LEU:HA	1.96	0.40
1:B:87:TRP:CE3	1:B:87:TRP:HA	2.56	0.40
1:A:196:ARG:H	1:A:196:ARG:HE	1.66	0.40
1:O:19:ARG:HD3	1:O:56:PHE:CD1	2.56	0.40
1:O:184:TYR:HD2	1:O:238:PRO:HA	1.87	0.40
1:P:159:CYS:HB2	1:P:294:SER:O	2.21	0.40

All (1) 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:B:84:ASN:O	4:A:387:HOH:O[3_555]	2.01	0.19

## 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	A	336/339 (99%)	306 (91%)	27 (8%)	3 (1%)	17	25
1	B	336/339 (99%)	317 (94%)	18 (5%)	1 (0%)	41	55
1	O	335/339 (99%)	311 (93%)	18 (5%)	6 (2%)	8	10
1	P	336/339 (99%)	305 (91%)	26 (8%)	5 (2%)	10	14
1	Q	336/339 (99%)	306 (91%)	27 (8%)	3 (1%)	17	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	336/339 (99%)	305 (91%)	24 (7%)	7 (2%)	7	8
All	All	2015/2034 (99%)	1850 (92%)	140 (7%)	25 (1%)	13	19

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	P	25	GLN
1	Q	174	ILE
1	R	337	TRP
1	O	54	GLY
1	P	192	ASP
1	P	203	ALA
1	R	172	GLY
1	A	172	GLY
1	B	242	VAL
1	O	55	ARG
1	O	203	ALA
1	O	242	VAL
1	P	242	VAL
1	Q	242	VAL
1	R	242	VAL
1	O	192	ASP
1	P	160	LEU
1	Q	192	ASP
1	A	203	ALA
1	O	172	GLY
1	R	38	SER
1	R	192	ASP
1	R	2	THR
1	R	67	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/284 (100%)	253 (89%)	31 (11%)	6	8
1	B	284/284 (100%)	255 (90%)	29 (10%)	7	10
1	O	283/284 (100%)	258 (91%)	25 (9%)	10	15
1	P	284/284 (100%)	249 (88%)	35 (12%)	4	6
1	Q	284/284 (100%)	234 (82%)	50 (18%)	2	2
1	R	284/284 (100%)	248 (87%)	36 (13%)	4	5
All	All	1703/1704 (100%)	1497 (88%)	206 (12%)	5	6

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	GLN
1	A	39	ASP
1	A	60	ILE
1	A	66	SER
1	A	77	VAL
1	A	95	VAL
1	A	97	GLU
1	A	109	SER
1	A	120	LEU
1	A	126	LYS
1	A	130	VAL
1	A	138	ASN
1	A	145	GLU
1	A	167	LEU
1	A	178	MET
1	A	186	LEU
1	A	190	ILE
1	A	196	ARG
1	A	209	VAL
1	A	231	ASN
1	A	242	VAL
1	A	251	VAL
1	A	260	VAL
1	A	286	SER
1	A	294	SER
1	A	303	LEU
1	A	309	LEU
1	A	326	VAL
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	336	LYS
1	B	1	MET
1	B	2	THR
1	B	18	LEU
1	B	39	ASP
1	B	65	ASN
1	B	77	VAL
1	B	79	ASP
1	B	80	ARG
1	B	87	TRP
1	B	88	LYS
1	B	97	GLU
1	B	101	VAL
1	B	119	VAL
1	B	120	LEU
1	B	126	LYS
1	B	130	VAL
1	B	167	LEU
1	B	175	LYS
1	B	189	ARG
1	B	196	ARG
1	B	198	LEU
1	B	199	ARG
1	B	209	VAL
1	B	219	VAL
1	B	260	VAL
1	B	266	LYS
1	B	305	MET
1	B	309	LEU
1	B	332	LEU
1	O	18	LEU
1	O	25	GLN
1	O	37	THR
1	O	38	SER
1	O	39	ASP
1	O	61	SER
1	O	67	ILE
1	O	83	LEU
1	O	87	TRP
1	O	88	LYS
1	O	109	SER
1	O	119	VAL

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Mol	Chain	Res	Type
1	O	120	LEU
1	O	139	ASP
1	O	167	LEU
1	O	178	MET
1	O	196	ARG
1	O	209	VAL
1	O	227	LYS
1	O	277	LYS
1	O	294	SER
1	O	300	SER
1	O	309	LEU
1	O	310	VAL
1	O	332	LEU
1	P	1	MET
1	P	2	THR
1	P	18	LEU
1	P	25	GLN
1	P	26	ASN
1	P	38	SER
1	P	39	ASP
1	P	41	ARG
1	P	60	ILE
1	P	61	SER
1	P	67	ILE
1	P	80	ARG
1	P	83	LEU
1	P	87	TRP
1	P	95	VAL
1	P	101	VAL
1	P	109	SER
1	P	113	GLN
1	P	119	VAL
1	P	120	LEU
1	P	145	GLU
1	P	146	ASP
1	P	167	LEU
1	P	178	MET
1	P	196	ARG
1	P	209	VAL
1	P	227	LYS
1	P	253	LYS
1	P	262	GLU

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Mol	Chain	Res	Type
1	P	295	SER
1	P	303	LEU
1	P	309	LEU
1	P	310	VAL
1	P	332	LEU
1	P	336	LYS
1	Q	1	MET
1	Q	2	THR
1	Q	7	ILE
1	Q	10	PHE
1	Q	18	LEU
1	Q	25	GLN
1	Q	32	VAL
1	Q	34	ILE
1	Q	41	ARG
1	Q	46	LEU
1	Q	59	ASP
1	Q	61	SER
1	Q	79	ASP
1	Q	83	LEU
1	Q	87	TRP
1	Q	95	VAL
1	Q	113	GLN
1	Q	118	LYS
1	Q	119	VAL
1	Q	126	LYS
1	Q	140	SER
1	Q	158	ASN
1	Q	175	LYS
1	Q	178	MET
1	Q	180	THR
1	Q	190	ILE
1	Q	194	SER
1	Q	196	ARG
1	Q	198	LEU
1	Q	199	ARG
1	Q	208	ILE
1	Q	209	VAL
1	Q	212	THR
1	Q	213	THR
1	Q	225	GLU
1	Q	227	LYS

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Mol	Chain	Res	Type
1	Q	260	VAL
1	Q	262	GLU
1	Q	266	LYS
1	Q	271	THR
1	Q	276	ILE
1	Q	295	SER
1	Q	300	SER
1	Q	303	LEU
1	Q	309	LEU
1	Q	310	VAL
1	Q	312	VAL
1	Q	318	ASN
1	Q	332	LEU
1	Q	335	ARG
1	R	2	THR
1	R	18	LEU
1	R	25	GLN
1	R	26	ASN
1	R	63	ASP
1	R	67	ILE
1	R	72	LYS
1	R	83	LEU
1	R	87	TRP
1	R	95	VAL
1	R	97	GLU
1	R	140	SER
1	R	141	GLU
1	R	151	SER
1	R	152	ASN
1	R	158	ASN
1	R	173	ILE
1	R	178	MET
1	R	180	THR
1	R	196	ARG
1	R	209	VAL
1	R	233	ILE
1	R	253	LYS
1	R	255	THR
1	R	256	ILE
1	R	259	GLN
1	R	262	GLU
1	R	263	VAL

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Mol	Chain	Res	Type
1	R	266	LYS
1	R	268	SER
1	R	294	SER
1	R	295	SER
1	R	302	THR
1	R	309	LEU
1	R	310	VAL
1	R	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	231	ASN
1	B	158	ASN
1	O	45	HIS
1	P	259	GLN
1	Q	144	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 ⓘ

18 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	6339	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	P	4340	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	O	3340	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	P	4339	-	4,4,4	0.27	0	6,6,6	0.17	0
3	NAD	R	340	-	42,48,48	1.31	3 (7%)	50,73,73	1.67	7 (14%)
2	SO4	Q	5339	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	Q	5340	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	A	1339	-	4,4,4	0.29	0	6,6,6	0.10	0
3	NAD	B	340	-	42,48,48	1.62	4 (9%)	50,73,73	1.38	5 (10%)
3	NAD	Q	340	-	42,48,48	1.40	4 (9%)	50,73,73	1.16	5 (10%)
2	SO4	O	3339	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	B	2340	-	4,4,4	0.28	0	6,6,6	0.13	0
3	NAD	A	340	-	42,48,48	1.50	4 (9%)	50,73,73	1.85	11 (22%)
3	NAD	P	340	-	42,48,48	1.45	5 (11%)	50,73,73	1.28	6 (12%)
3	NAD	O	340	-	42,48,48	1.46	4 (9%)	50,73,73	1.59	8 (16%)
2	SO4	B	2339	-	4,4,4	0.39	0	6,6,6	0.31	0
2	SO4	A	1340	-	4,4,4	0.28	0	6,6,6	0.25	0
2	SO4	R	6340	-	4,4,4	0.31	0	6,6,6	0.11	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	R	340	-	-	13/26/62/62	0/5/5/5
3	NAD	B	340	-	-	12/26/62/62	0/5/5/5
3	NAD	Q	340	-	-	7/26/62/62	0/5/5/5
3	NAD	A	340	-	-	9/26/62/62	0/5/5/5
3	NAD	P	340	-	-	12/26/62/62	0/5/5/5
3	NAD	O	340	-	-	12/26/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	340	NAD	PN-O3	5.37	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	340	NAD	O4D-C1D	4.67	1.47	1.40
3	A	340	NAD	O4B-C1B	4.48	1.46	1.40
3	B	340	NAD	O4B-C1B	4.48	1.46	1.40
3	Q	340	NAD	O4D-C1D	4.15	1.46	1.40
3	P	340	NAD	PN-O3	4.15	1.64	1.59
3	B	340	NAD	O4D-C1D	4.14	1.46	1.40
3	O	340	NAD	O4B-C1B	4.04	1.46	1.40
3	A	340	NAD	PN-O3	4.03	1.63	1.59
3	P	340	NAD	O4D-C1D	3.88	1.46	1.40
3	R	340	NAD	O4B-C1B	3.86	1.46	1.40
3	O	340	NAD	O4D-C1D	3.84	1.45	1.40
3	O	340	NAD	PN-O3	3.81	1.63	1.59
3	P	340	NAD	O4B-C1B	3.78	1.45	1.40
3	Q	340	NAD	O4B-C1B	3.66	1.45	1.40
3	R	340	NAD	PN-O3	3.58	1.63	1.59
3	R	340	NAD	O4D-C1D	3.49	1.45	1.40
3	B	340	NAD	PA-O3	3.46	1.63	1.59
3	P	340	NAD	PA-O3	3.28	1.63	1.59
3	O	340	NAD	PA-O3	3.21	1.63	1.59
3	Q	340	NAD	PN-O3	3.07	1.62	1.59
3	Q	340	NAD	PA-O3	3.06	1.62	1.59
3	P	340	NAD	C8A-N7A	-2.41	1.30	1.34
3	A	340	NAD	C8A-N7A	-2.22	1.30	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	340	NAD	C4B-O4B-C1B	-7.58	102.99	109.92
3	R	340	NAD	C4B-O4B-C1B	-7.21	103.32	109.92
3	A	340	NAD	N3A-C2A-N1A	-5.24	121.56	128.67
3	O	340	NAD	C4B-O4B-C1B	-4.93	105.41	109.92
3	O	340	NAD	N3A-C2A-N1A	-4.75	122.23	128.67
3	R	340	NAD	N3A-C2A-N1A	-4.52	122.53	128.67
3	Q	340	NAD	N3A-C2A-N1A	-4.51	122.55	128.67
3	B	340	NAD	N3A-C2A-N1A	-4.47	122.60	128.67
3	P	340	NAD	N3A-C2A-N1A	-4.36	122.75	128.67
3	B	340	NAD	C5N-C4N-C3N	-3.48	116.95	120.36
3	O	340	NAD	O2N-PN-O3	3.25	116.06	107.27
3	A	340	NAD	O2N-PN-O3	3.01	115.42	107.27
3	P	340	NAD	C4B-O4B-C1B	-2.88	107.29	109.92
3	R	340	NAD	C5N-C4N-C3N	-2.87	117.54	120.36
3	A	340	NAD	C5N-C4N-C3N	-2.79	117.62	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	340	NAD	C4A-C5A-N7A	-2.79	106.39	109.34
3	B	340	NAD	C4A-C5A-N7A	-2.77	106.41	109.34
3	O	340	NAD	O4B-C4B-C5B	2.75	118.15	109.33
3	Q	340	NAD	C5N-C4N-C3N	-2.74	117.67	120.36
3	P	340	NAD	C5D-C4D-C3D	-2.74	105.35	115.21
3	B	340	NAD	O5B-C5B-C4B	2.72	118.24	108.99
3	O	340	NAD	C5N-C4N-C3N	-2.68	117.73	120.36
3	A	340	NAD	O4B-C1B-N9A	2.65	112.25	108.75
3	B	340	NAD	PA-O5B-C5B	-2.64	106.24	121.35
3	R	340	NAD	O2N-PN-O3	2.58	114.25	107.27
3	O	340	NAD	C3N-C7N-N7N	2.43	120.73	117.74
3	O	340	NAD	O4B-C1B-N9A	2.42	111.96	108.75
3	A	340	NAD	O2A-PA-O3	2.36	113.65	107.27
3	P	340	NAD	PA-O5B-C5B	-2.36	107.85	121.35
3	A	340	NAD	PA-O5B-C5B	-2.32	108.07	121.35
3	O	340	NAD	C4A-C5A-N7A	-2.30	106.90	109.34
3	P	340	NAD	C5N-C4N-C3N	-2.29	118.12	120.36
3	Q	340	NAD	PA-O5B-C5B	-2.25	108.45	121.35
3	A	340	NAD	O7N-C7N-N7N	-2.23	119.40	122.62
3	A	340	NAD	O4B-C4B-C5B	2.18	116.32	109.33
3	A	340	NAD	O3-PA-O1A	-2.13	104.30	110.70
3	Q	340	NAD	C4A-C5A-N7A	-2.11	107.11	109.34
3	Q	340	NAD	C5B-C4B-C3B	-2.09	107.69	115.21
3	P	340	NAD	O2N-PN-O3	2.07	112.88	107.27
3	A	340	NAD	C4A-C5A-N7A	-2.05	107.17	109.34
3	R	340	NAD	O4B-C1B-N9A	2.04	111.45	108.75
3	R	340	NAD	PA-O5B-C5B	-2.01	109.85	121.35

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	340	NAD	C5B-O5B-PA-O1A
3	A	340	NAD	C5B-O5B-PA-O2A
3	A	340	NAD	C5B-O5B-PA-O3
3	A	340	NAD	C5D-O5D-PN-O3
3	A	340	NAD	O4D-C1D-N1N-C2N
3	A	340	NAD	O4D-C1D-N1N-C6N
3	B	340	NAD	C5B-O5B-PA-O1A
3	B	340	NAD	C5B-O5B-PA-O3
3	B	340	NAD	O4D-C1D-N1N-C2N
3	B	340	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	O	340	NAD	C5B-O5B-PA-O1A
3	O	340	NAD	C5B-O5B-PA-O2A
3	O	340	NAD	C5B-O5B-PA-O3
3	O	340	NAD	C5D-O5D-PN-O3
3	O	340	NAD	C5D-O5D-PN-O1N
3	O	340	NAD	C5D-O5D-PN-O2N
3	O	340	NAD	O4D-C1D-N1N-C2N
3	O	340	NAD	O4D-C1D-N1N-C6N
3	O	340	NAD	C2D-C1D-N1N-C2N
3	O	340	NAD	C2D-C1D-N1N-C6N
3	P	340	NAD	C5B-O5B-PA-O1A
3	P	340	NAD	C5B-O5B-PA-O2A
3	P	340	NAD	C5B-O5B-PA-O3
3	P	340	NAD	O4D-C1D-N1N-C2N
3	P	340	NAD	O4D-C1D-N1N-C6N
3	Q	340	NAD	C5D-O5D-PN-O1N
3	Q	340	NAD	O4D-C1D-N1N-C2N
3	R	340	NAD	C5B-O5B-PA-O1A
3	R	340	NAD	C5B-O5B-PA-O2A
3	R	340	NAD	C5B-O5B-PA-O3
3	R	340	NAD	O4D-C1D-N1N-C2N
3	R	340	NAD	O4D-C1D-N1N-C6N
3	R	340	NAD	C2D-C1D-N1N-C2N
3	R	340	NAD	C2D-C1D-N1N-C6N
3	R	340	NAD	C2N-C3N-C7N-O7N
3	R	340	NAD	C2N-C3N-C7N-N7N
3	R	340	NAD	C4N-C3N-C7N-O7N
3	R	340	NAD	C4N-C3N-C7N-N7N
3	B	340	NAD	O4B-C4B-C5B-O5B
3	P	340	NAD	O4B-C4B-C5B-O5B
3	Q	340	NAD	O4B-C4B-C5B-O5B
3	P	340	NAD	C3B-C4B-C5B-O5B
3	Q	340	NAD	C3B-C4B-C5B-O5B
3	B	340	NAD	C3B-C4B-C5B-O5B
3	P	340	NAD	PA-O3-PN-O1N
3	P	340	NAD	PN-O3-PA-O5B
3	Q	340	NAD	O4D-C4D-C5D-O5D
3	B	340	NAD	C5B-O5B-PA-O2A
3	B	340	NAD	C5D-O5D-PN-O3
3	B	340	NAD	C5D-O5D-PN-O2N
3	P	340	NAD	C5D-O5D-PN-O1N
3	A	340	NAD	PA-O3-PN-O1N

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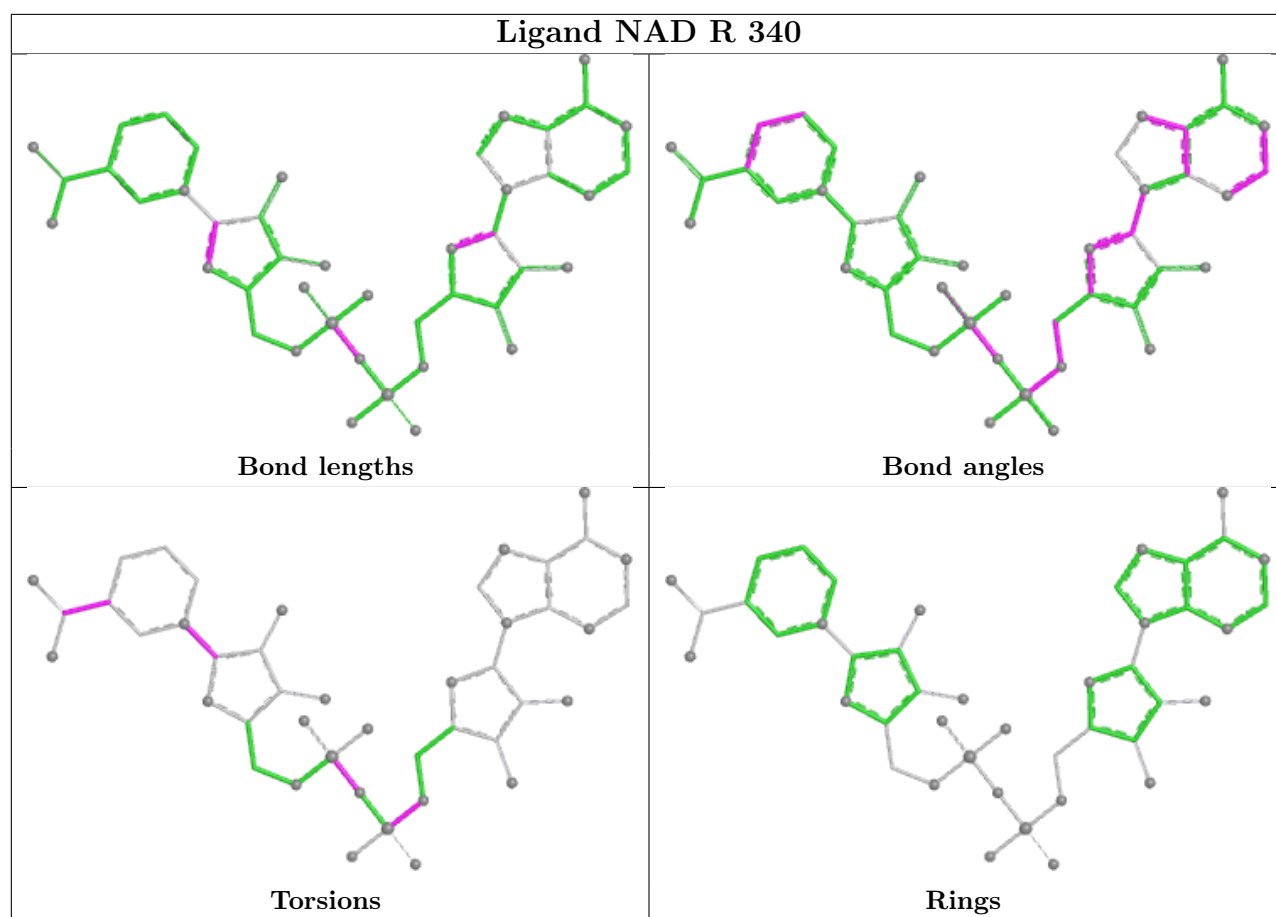
Mol	Chain	Res	Type	Atoms
3	A	340	NAD	PA-O3-PN-O2N
3	B	340	NAD	PA-O3-PN-O1N
3	O	340	NAD	PA-O3-PN-O2N
3	B	340	NAD	C4B-C5B-O5B-PA
3	A	340	NAD	C2D-C1D-N1N-C6N
3	B	340	NAD	C2D-C1D-N1N-C6N
3	P	340	NAD	C2D-C1D-N1N-C6N
3	Q	340	NAD	O4D-C1D-N1N-C6N
3	R	340	NAD	PA-O3-PN-O2N
3	O	340	NAD	PA-O3-PN-O1N
3	P	340	NAD	PA-O3-PN-O2N
3	R	340	NAD	PA-O3-PN-O1N
3	Q	340	NAD	C3D-C4D-C5D-O5D

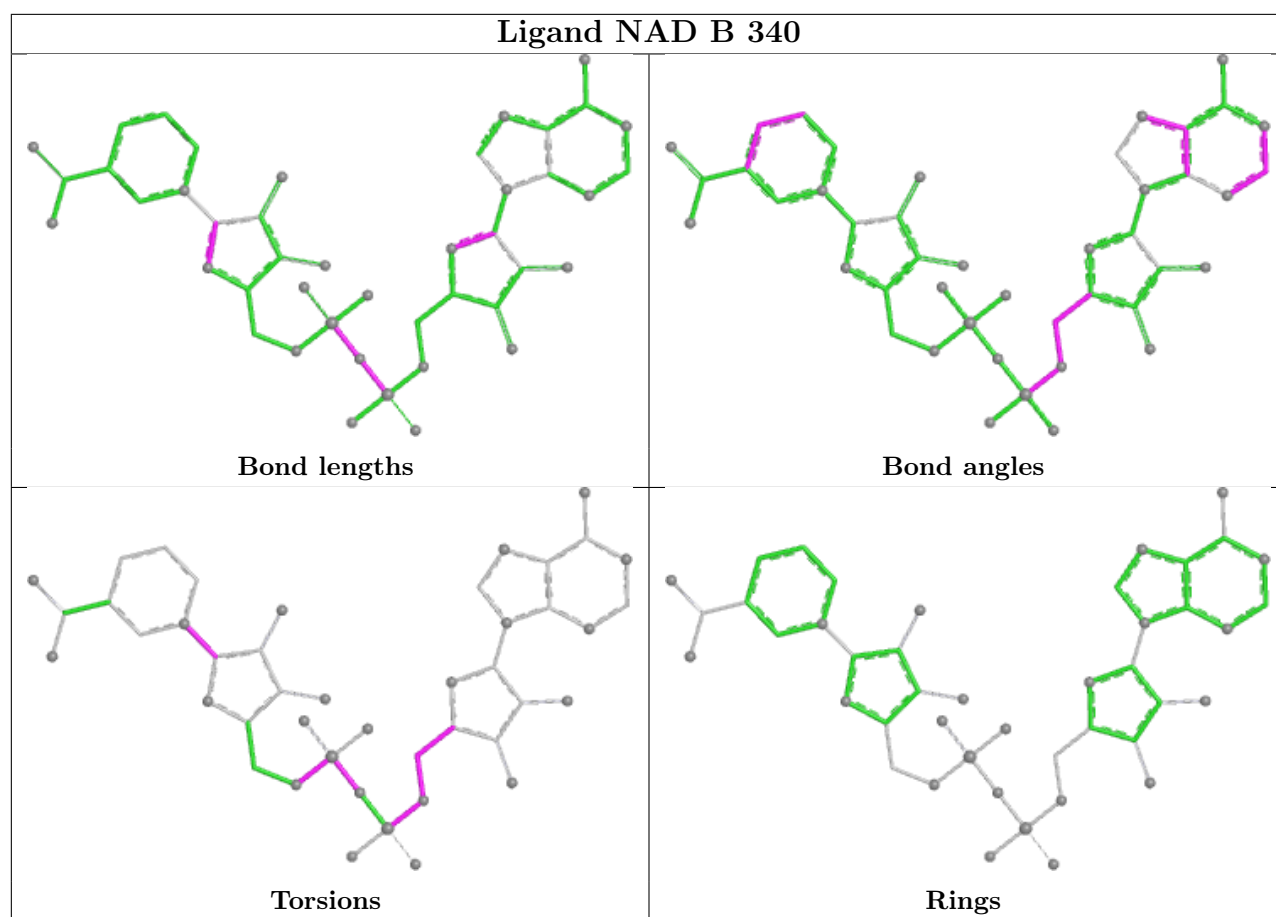
There are no ring outliers.

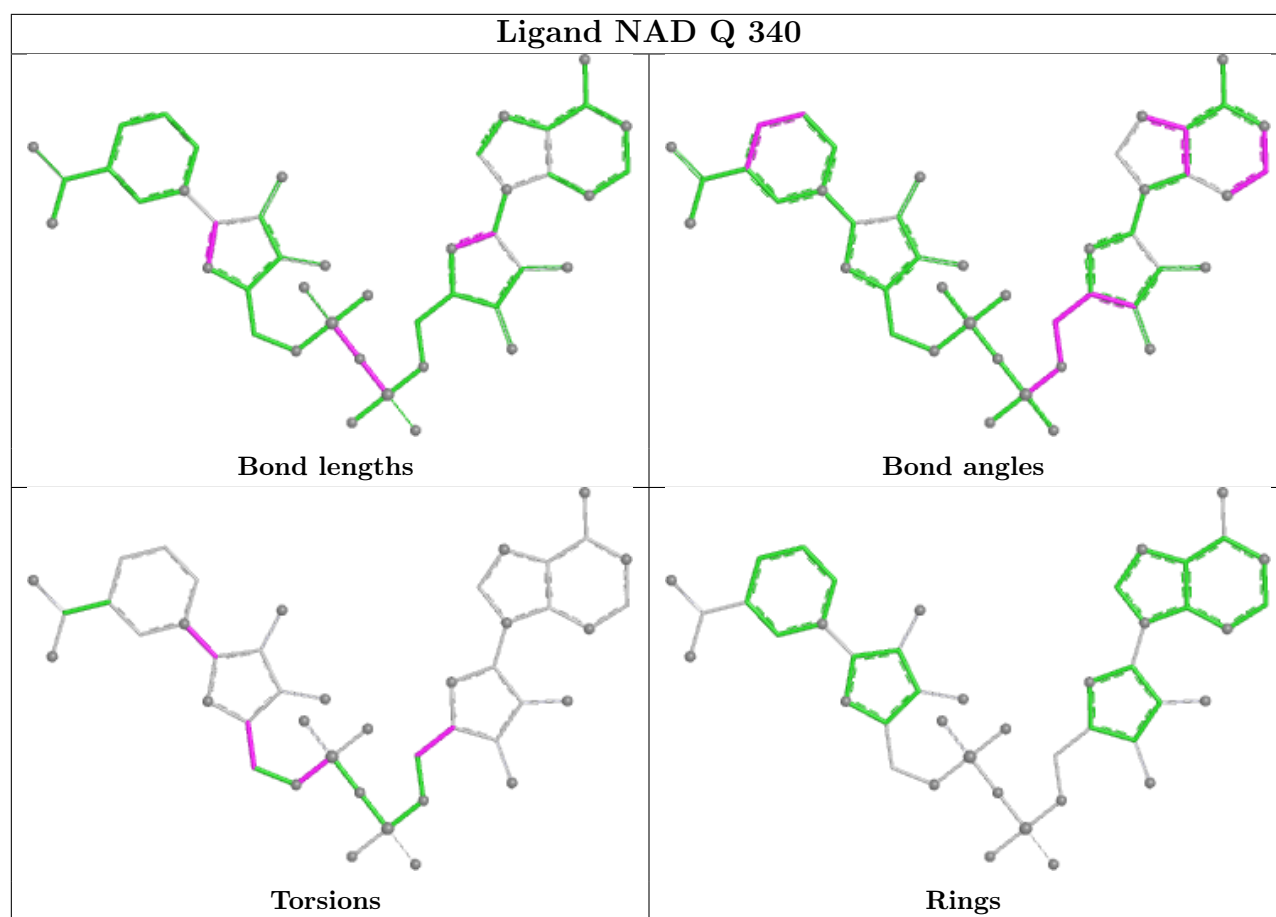
7 monomers are involved in 28 short contacts:

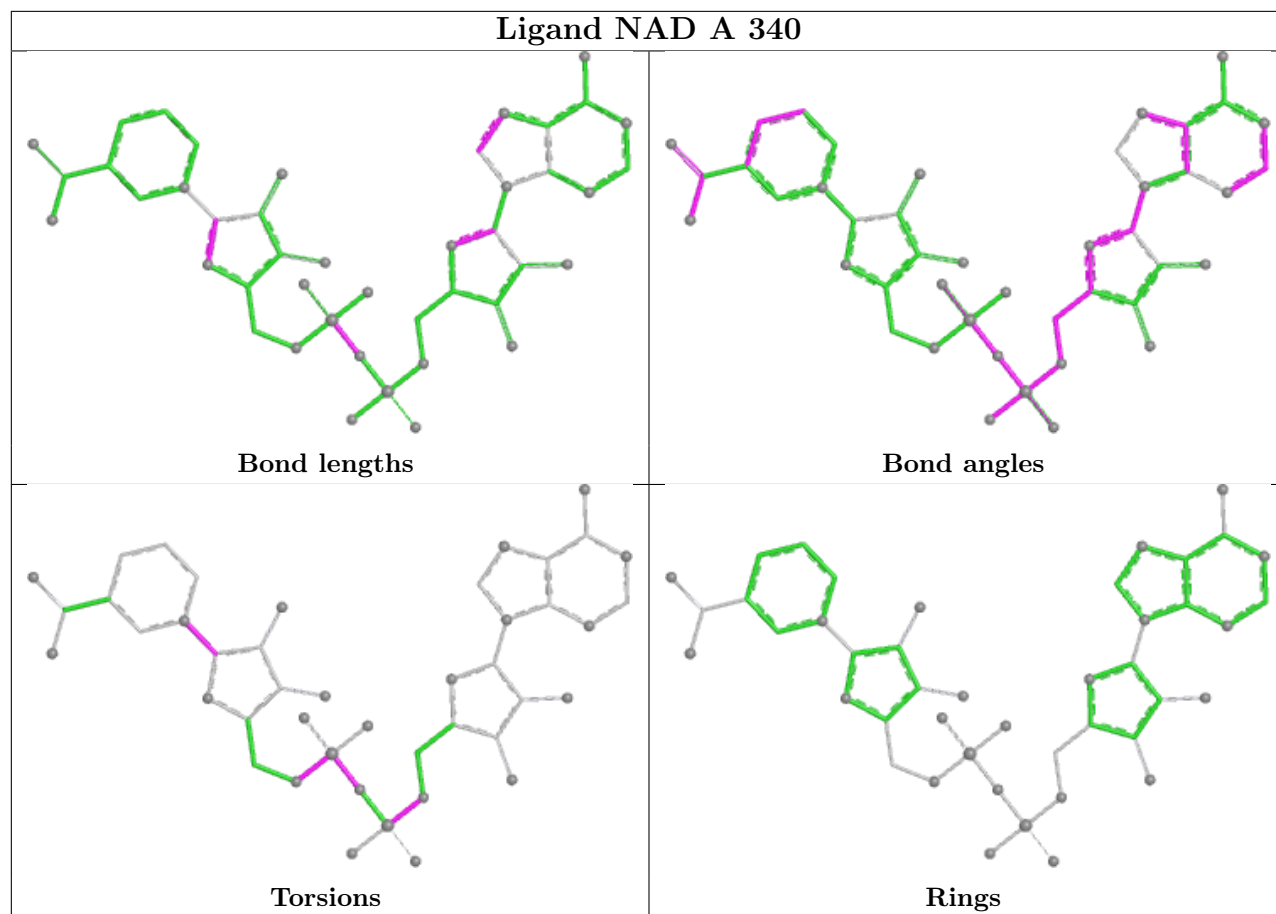
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	340	NAD	5	0
3	B	340	NAD	5	0
3	Q	340	NAD	2	0
2	O	3339	SO4	1	0
3	A	340	NAD	7	0
3	P	340	NAD	4	0
3	O	340	NAD	4	0

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.

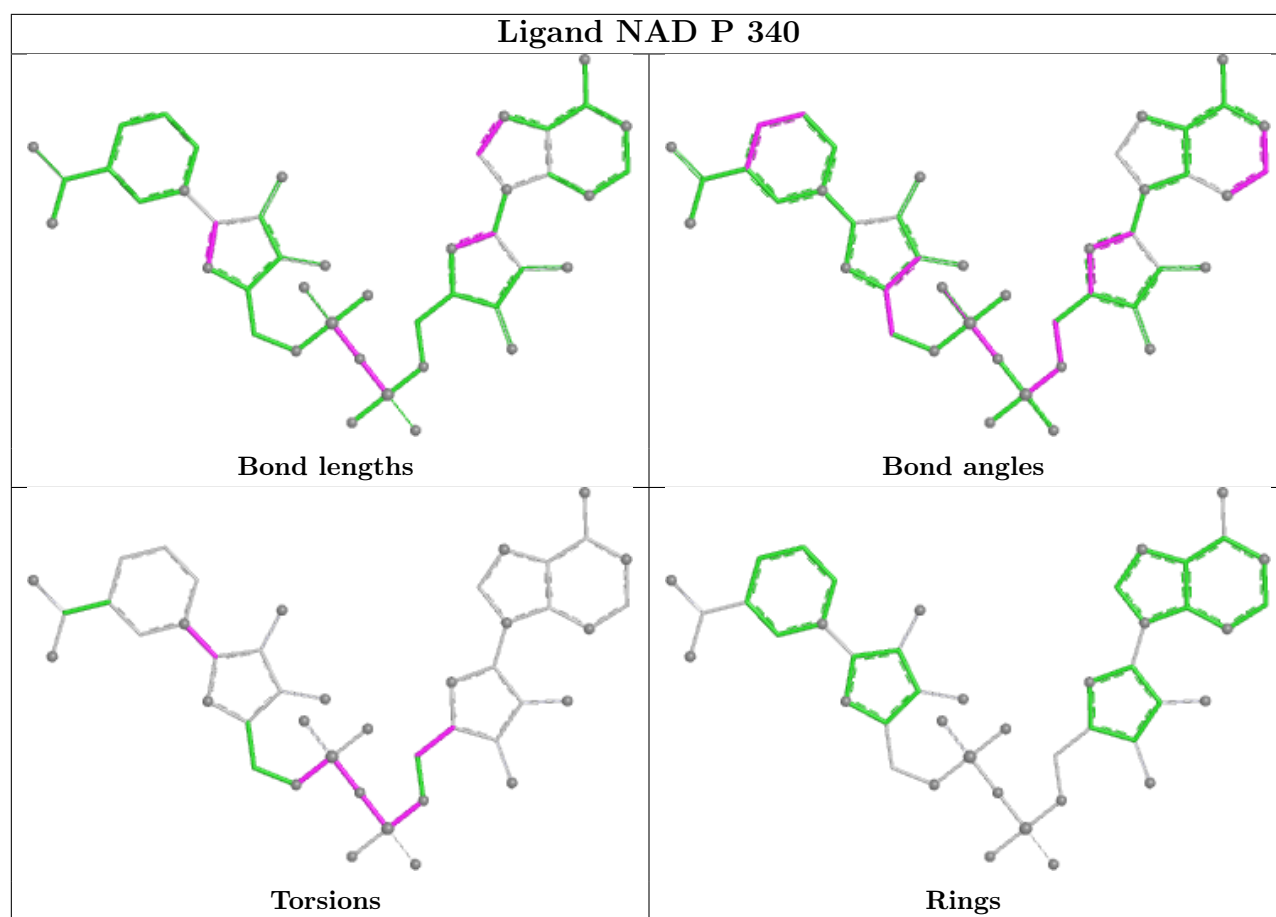


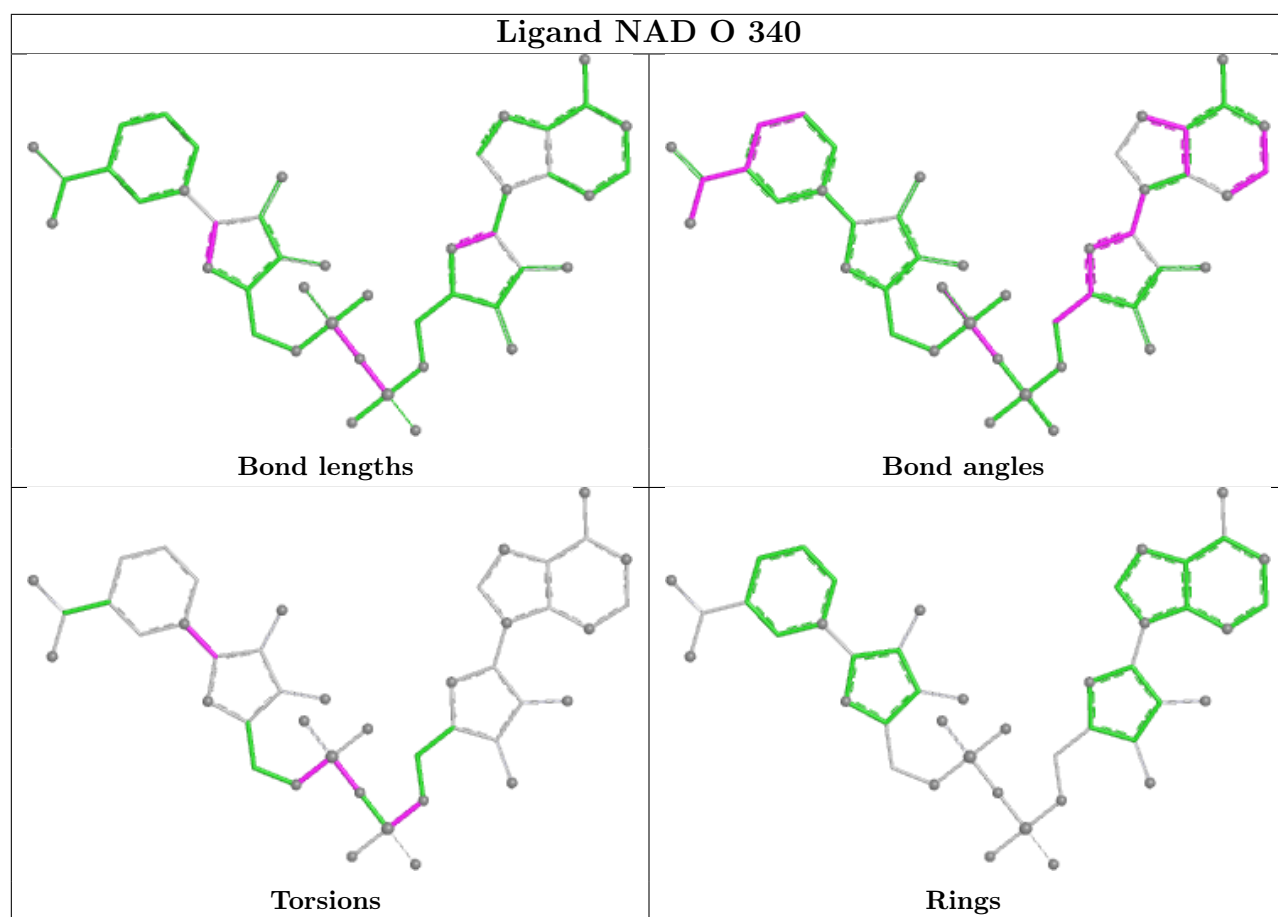












## 5.7 Other polymers [i](#)

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	A	338/339 (99%)	0.59	27 (7%)	12 11	28, 43, 64, 85	0
1	B	338/339 (99%)	0.28	4 (1%)	79 77	28, 40, 55, 70	0
1	O	337/339 (99%)	0.44	7 (2%)	63 61	30, 44, 62, 75	0
1	P	338/339 (99%)	0.82	47 (13%)	2 2	32, 48, 73, 95	0
1	Q	338/339 (99%)	1.10	67 (19%)	1 0	48, 65, 83, 99	0
1	R	338/339 (99%)	1.04	57 (16%)	1 1	45, 60, 75, 89	0
All	All	2027/2034 (99%)	0.71	209 (10%)	6 6	28, 51, 75, 99	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	60	ILE	8.0
1	P	1	MET	7.0
1	A	67	ILE	6.3
1	B	1	MET	6.0
1	Q	1	MET	6.0
1	R	61	SER	5.8
1	A	1	MET	5.4
1	P	67	ILE	5.4
1	R	66	SER	5.2
1	A	61	SER	5.2
1	A	60	ILE	5.1
1	R	67	ILE	5.0
1	R	1	MET	4.9
1	A	64	GLU	4.9
1	A	65	ASN	4.8
1	P	69	VAL	4.8
1	P	90	TRP	4.6
1	P	36	ASN	4.4
1	R	42	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	Q	90	TRP	4.3
1	R	249	VAL	4.2
1	O	193	ALA	4.2
1	P	65	ASN	4.2
1	R	259	GLN	4.1
1	R	64	GLU	4.1
1	A	68	THR	4.1
1	R	62	TYR	4.1
1	O	71	GLY	4.1
1	R	63	ASP	4.0
1	Q	63	ASP	4.0
1	Q	338	ALA	4.0
1	P	77	VAL	4.0
1	Q	62	TYR	3.9
1	R	310	VAL	3.9
1	Q	69	VAL	3.9
1	Q	26	ASN	3.9
1	P	80	ARG	3.9
1	R	167	LEU	3.9
1	R	43	ALA	3.8
1	Q	303	LEU	3.8
1	R	65	ASN	3.8
1	R	173	ILE	3.8
1	P	64	GLU	3.8
1	Q	266	LYS	3.7
1	R	76	ILE	3.7
1	Q	74	MET	3.7
1	A	43	ALA	3.7
1	A	62	TYR	3.7
1	P	45	HIS	3.6
1	Q	56	PHE	3.6
1	A	42	THR	3.6
1	R	75	LYS	3.6
1	R	239	THR	3.6
1	A	71	GLY	3.5
1	R	238	PRO	3.5
1	R	37	THR	3.5
1	Q	72	LYS	3.5
1	P	92	ILE	3.5
1	R	237	VAL	3.5
1	R	41	ARG	3.5
1	Q	58	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	Q	59	ASP	3.4
1	O	194	SER	3.4
1	P	43	ALA	3.4
1	P	61	SER	3.4
1	Q	309	LEU	3.4
1	Q	43	ALA	3.4
1	Q	67	ILE	3.4
1	R	69	VAL	3.4
1	A	74	MET	3.4
1	Q	240	PRO	3.4
1	P	32	VAL	3.3
1	O	73	THR	3.3
1	R	73	THR	3.3
1	P	42	THR	3.3
1	A	63	ASP	3.3
1	P	206	VAL	3.3
1	Q	239	THR	3.3
1	P	338	ALA	3.3
1	Q	206	VAL	3.3
1	Q	254	PRO	3.2
1	P	95	VAL	3.2
1	P	62	TYR	3.2
1	Q	64	GLU	3.2
1	A	90	TRP	3.1
1	R	223	ILE	3.1
1	R	254	PRO	3.1
1	A	72	LYS	3.1
1	Q	262	GLU	3.1
1	Q	65	ASN	3.1
1	R	171	PHE	3.1
1	R	305	MET	3.1
1	A	69	VAL	3.0
1	P	83	LEU	3.0
1	Q	29	LEU	3.0
1	R	252	GLU	3.0
1	Q	70	ASN	3.0
1	A	76	ILE	3.0
1	R	166	VAL	3.0
1	P	41	ARG	3.0
1	O	206	VAL	2.9
1	P	81	ASN	2.9
1	R	304	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	66	SER	2.9
1	Q	27	THR	2.9
1	Q	166	VAL	2.9
1	Q	269	GLN	2.9
1	Q	83	LEU	2.9
1	Q	71	GLY	2.9
1	A	73	THR	2.9
1	O	239	THR	2.9
1	P	74	MET	2.9
1	P	204	ALA	2.9
1	P	203	ALA	2.8
1	P	66	SER	2.8
1	R	174	ILE	2.8
1	P	101	VAL	2.8
1	R	5	VAL	2.8
1	R	68	THR	2.8
1	P	78	CYS	2.8
1	P	84	ASN	2.7
1	P	22	PHE	2.7
1	R	260	VAL	2.7
1	A	36	ASN	2.6
1	Q	73	THR	2.6
1	R	206	VAL	2.6
1	Q	60	ILE	2.6
1	Q	304	VAL	2.6
1	Q	68	THR	2.6
1	Q	237	VAL	2.6
1	R	209	VAL	2.6
1	B	190	ILE	2.6
1	Q	273	LYS	2.6
1	Q	238	PRO	2.6
1	P	60	ILE	2.6
1	P	38	SER	2.5
1	Q	174	ILE	2.5
1	Q	223	ILE	2.5
1	P	34	ILE	2.5
1	R	208	ILE	2.5
1	Q	31	VAL	2.5
1	Q	30	GLU	2.5
1	R	59	ASP	2.5
1	Q	204	ALA	2.4
1	R	203	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	75	LYS	2.4
1	R	271	THR	2.4
1	R	258	GLU	2.4
1	P	119	VAL	2.4
1	P	2	THR	2.4
1	R	226	LEU	2.4
1	Q	252	GLU	2.4
1	Q	78	CYS	2.4
1	P	238	PRO	2.3
1	R	31	VAL	2.3
1	Q	32	VAL	2.3
1	P	240	PRO	2.3
1	Q	185	THR	2.3
1	P	87	TRP	2.3
1	R	253	LYS	2.3
1	A	44	ALA	2.3
1	A	37	THR	2.3
1	A	32	VAL	2.3
1	A	242	VAL	2.3
1	R	182	HIS	2.3
1	Q	184	TYR	2.2
1	P	63	ASP	2.2
1	B	263	VAL	2.2
1	O	64	GLU	2.2
1	R	309	LEU	2.2
1	R	240	PRO	2.2
1	Q	61	SER	2.2
1	Q	76	ILE	2.2
1	Q	25	GLN	2.2
1	Q	4	ARG	2.2
1	Q	180	THR	2.2
1	Q	253	LYS	2.2
1	Q	305	MET	2.2
1	R	74	MET	2.2
1	R	95	VAL	2.2
1	Q	203	ALA	2.2
1	R	80	ARG	2.2
1	Q	155	CYS	2.2
1	R	90	TRP	2.2
1	P	89	GLU	2.2
1	Q	55	ARG	2.1
1	A	203	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	9	GLY	2.1
1	P	58	ALA	2.1
1	Q	243	SER	2.1
1	P	23	GLY	2.1
1	P	205	ALA	2.1
1	P	330	ALA	2.1
1	Q	42	THR	2.1
1	R	270	THR	2.1
1	Q	251	VAL	2.1
1	R	262	GLU	2.1
1	Q	88	LYS	2.1
1	A	80	ARG	2.1
1	B	270	THR	2.1
1	Q	244	VAL	2.1
1	P	39	ASP	2.0
1	R	251	VAL	2.0
1	P	102	PHE	2.0
1	A	75	LYS	2.0
1	R	83	LEU	2.0
1	Q	2	THR	2.0
1	Q	5	VAL	2.0
1	Q	48	GLU	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( $\text{\AA}^2$ )	Q<0.9
3	NAD	P	340	44/44	0.87	0.18	51,63,70,71	0

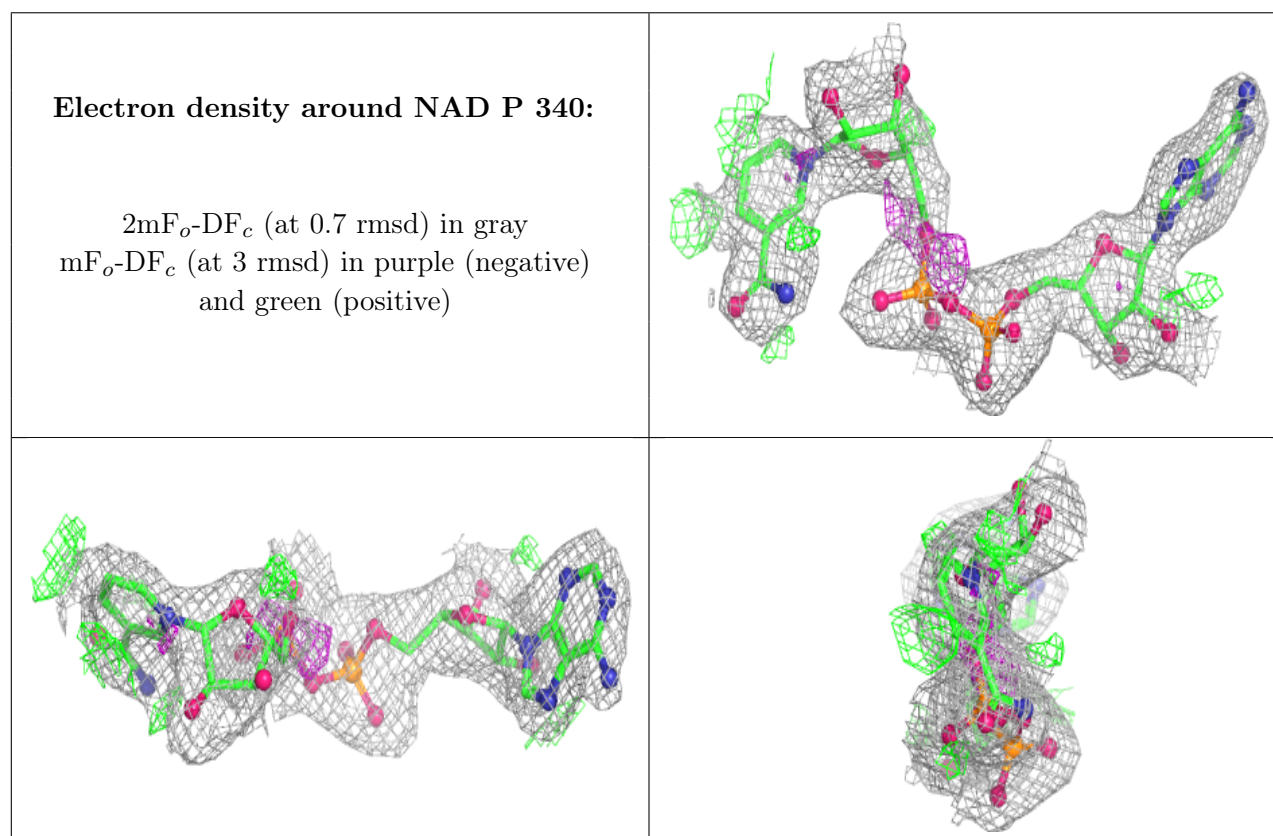
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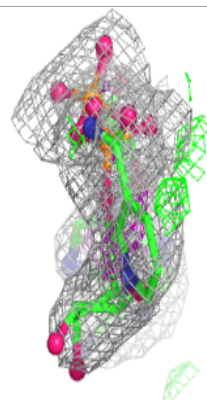
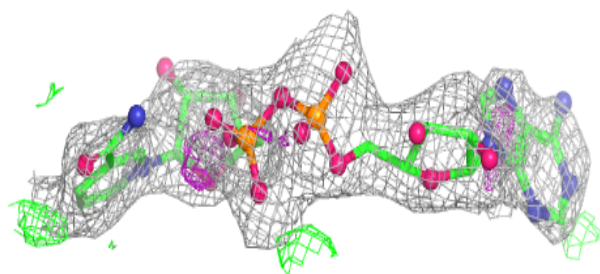
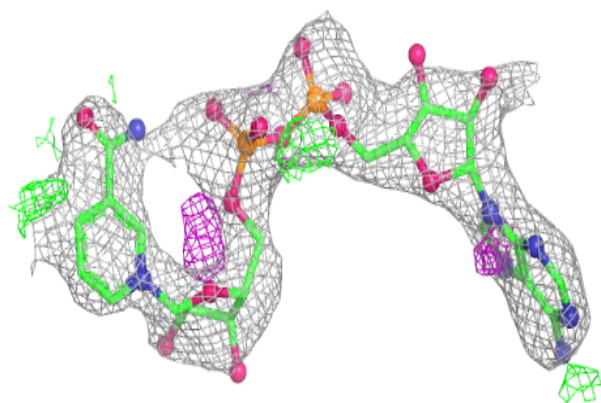
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	Q	340	44/44	0.87	0.20	63,73,77,79	0
3	NAD	R	340	44/44	0.89	0.25	56,68,73,74	0
2	SO4	R	6340	5/5	0.90	0.16	72,74,76,80	5
2	SO4	O	3340	5/5	0.91	0.20	66,66,73,73	5
2	SO4	Q	5339	5/5	0.91	0.20	65,68,75,77	5
2	SO4	P	4340	5/5	0.92	0.19	66,68,73,77	5
3	NAD	A	340	44/44	0.93	0.16	39,51,58,59	0
2	SO4	Q	5340	5/5	0.93	0.21	71,77,81,82	5
3	NAD	O	340	44/44	0.94	0.14	42,51,58,60	0
3	NAD	B	340	44/44	0.94	0.15	32,46,52,55	0
2	SO4	R	6339	5/5	0.95	0.13	65,65,74,78	0
2	SO4	A	1340	5/5	0.95	0.22	55,56,58,60	5
2	SO4	B	2340	5/5	0.96	0.18	53,57,59,60	5
2	SO4	P	4339	5/5	0.97	0.20	42,45,50,53	0
2	SO4	O	3339	5/5	0.98	0.15	41,44,50,51	5
2	SO4	B	2339	5/5	0.98	0.14	42,43,51,54	0
2	SO4	A	1339	5/5	0.99	0.15	36,38,47,48	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.

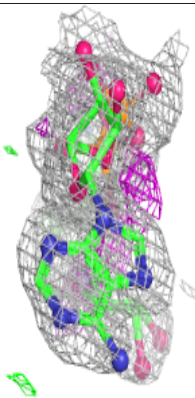
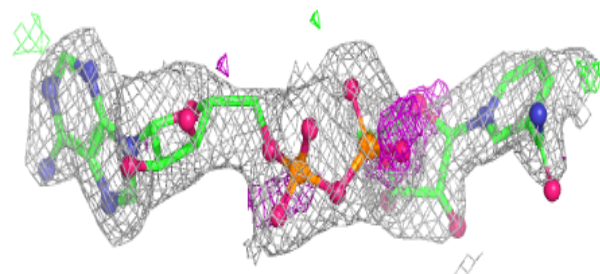
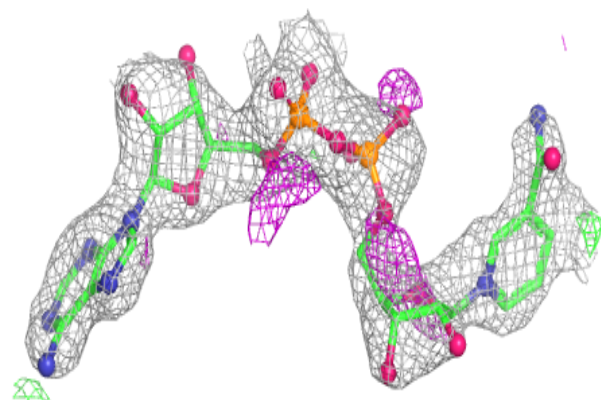


**Electron density around NAD Q 340:**

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

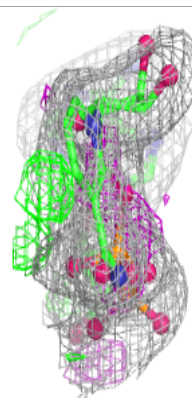
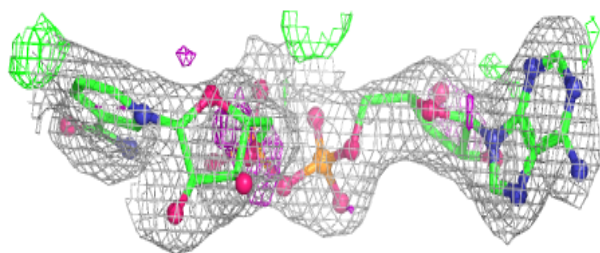
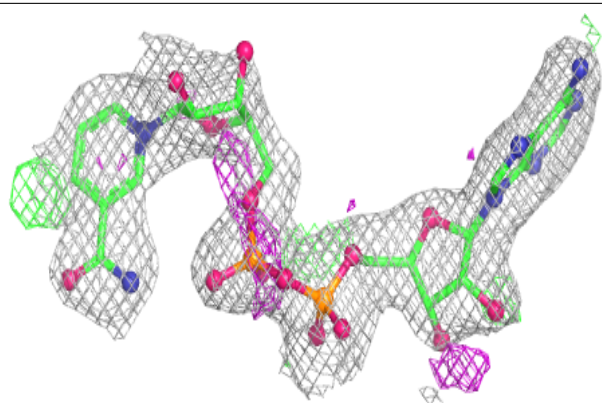
**Electron density around NAD R 340:**

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

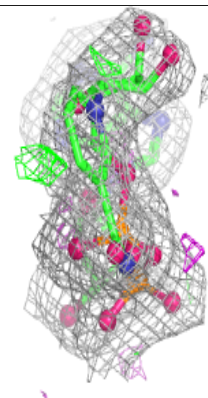
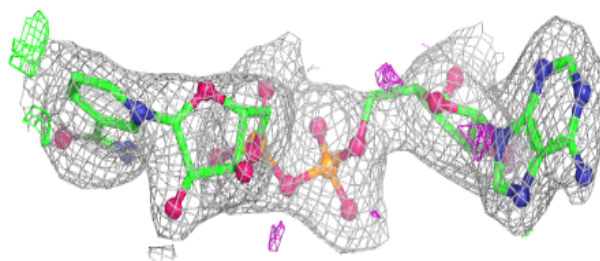
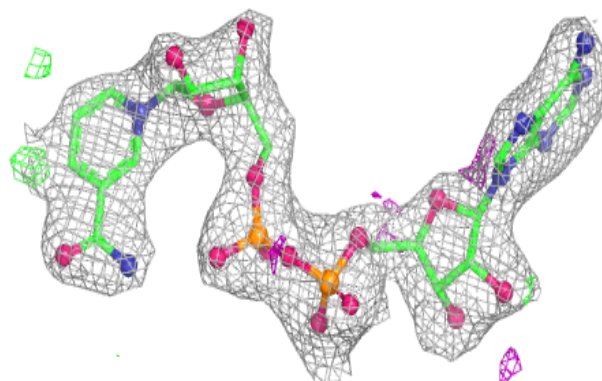


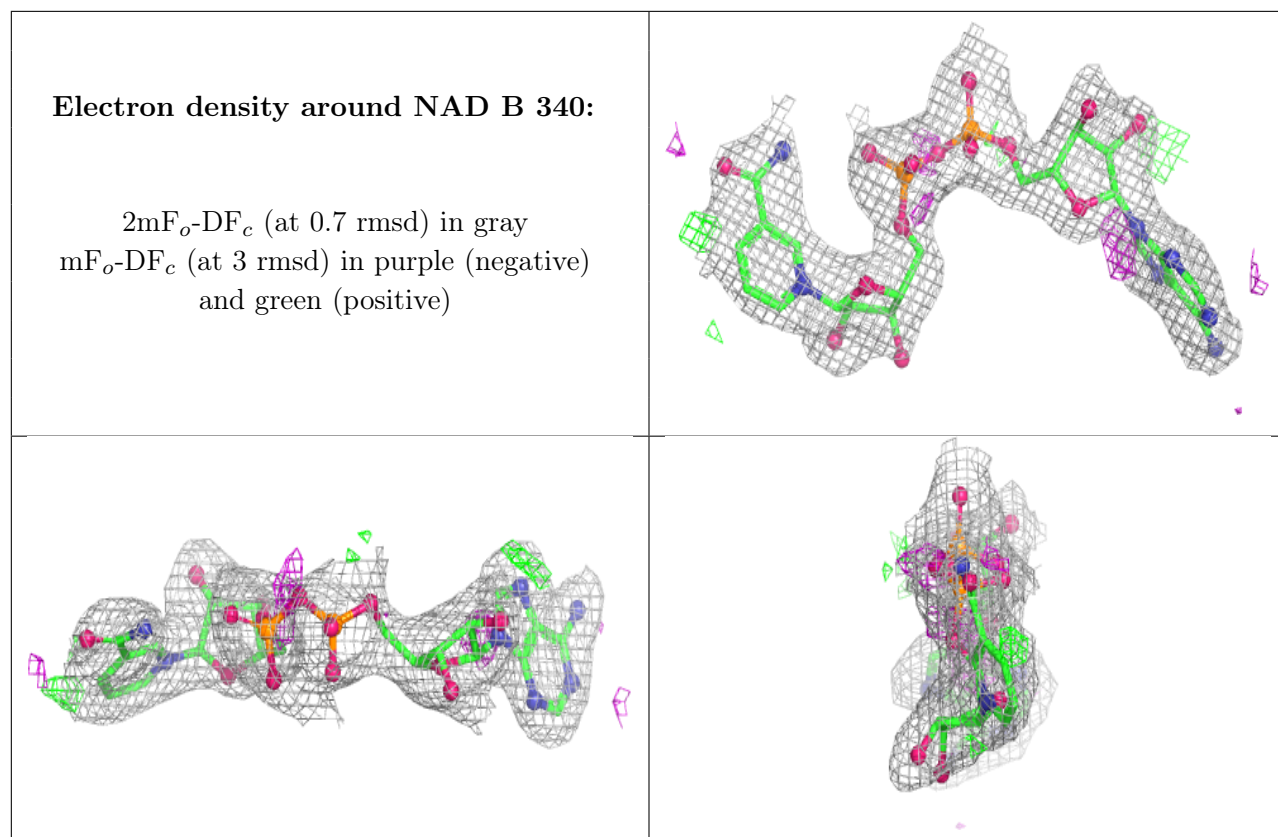
**Electron density around NAD A 340:**

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

**Electron density around NAD O 340:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.