



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:03 AM UTC

PDB ID : 1GZF / pdb_00001gzf
Title : Structure of the Clostridium botulinum C3 exoenzyme (wild-type) in complex with NAD
Authors : Menetrey, J.; Flatau, G.; Stura, E.A.; Charbonnier, J.B.; Gas, F.; Teulon, J.M.; Le Du, M.H.; Boquet, P.; Menez, A.
Deposited on : 2002-05-21
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

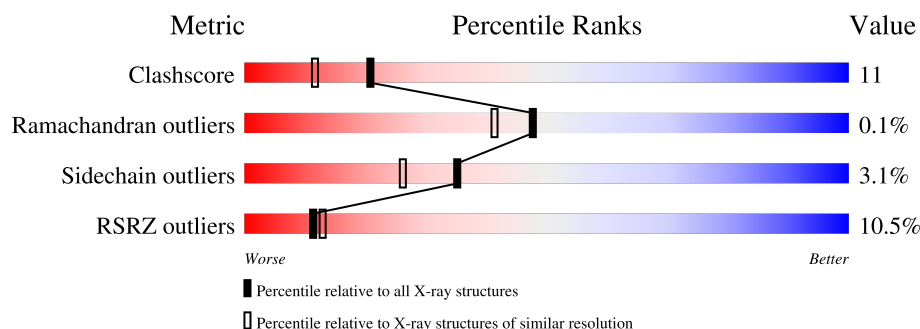
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	4% 73% 22% .
1	B	211	18% 72% 25% .
1	C	211	10% 76% 21% ..
1	D	211	9% 69% 25% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

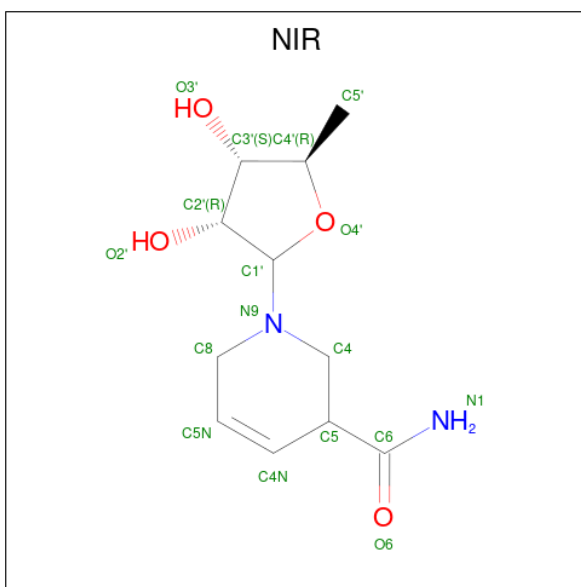
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	A	1248	X	-	-	-
2	NAD	B	1252	X	-	-	-
4	NIR	C	1252	X	-	-	-

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



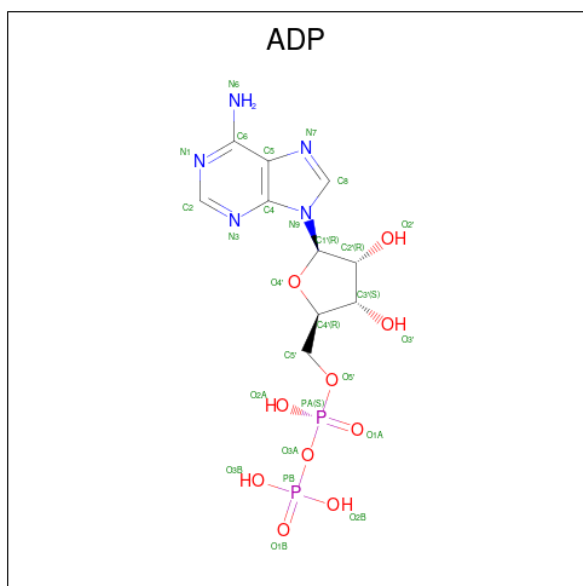
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 3-(AMINOCARBONYL)-1-[(3R,4S,5R)-3,4-DIHYDROXY-5-METHYLTETRAHYDRO-2-FURANYL]PYRIDINIUM (CCD ID: NIR) (formula: C₁₁H₁₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			17	11	2	4		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

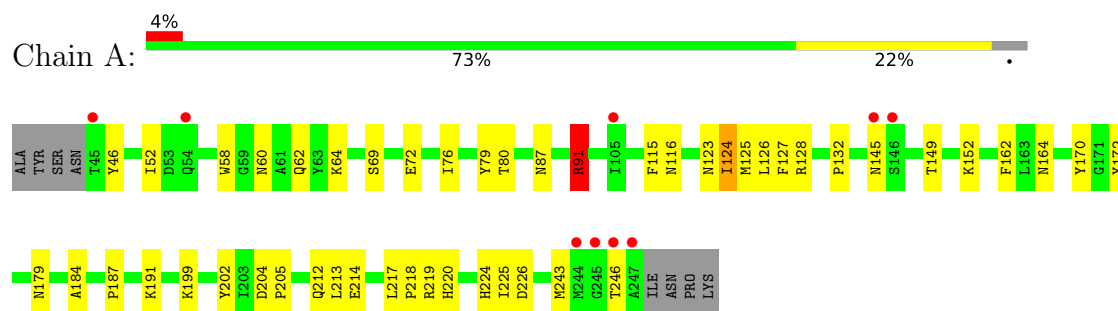
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	168	Total	O	0	0
			168	168		
6	B	125	Total	O	0	0
			125	125		
6	C	139	Total	O	0	0
			139	139		
6	D	138	Total	O	0	0
			138	138		

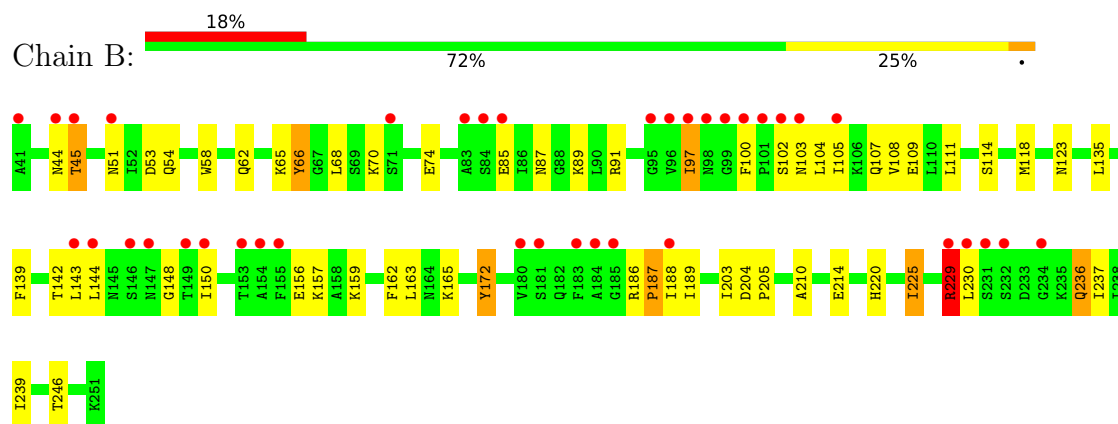
3 Residue-property plots [i](#)

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.

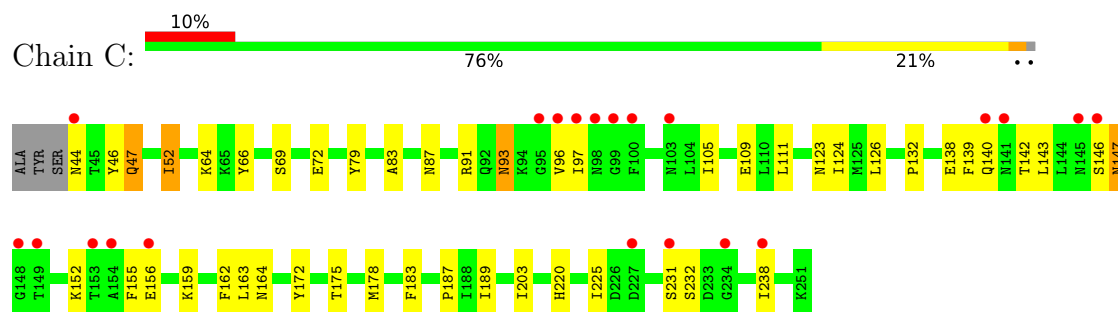
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3



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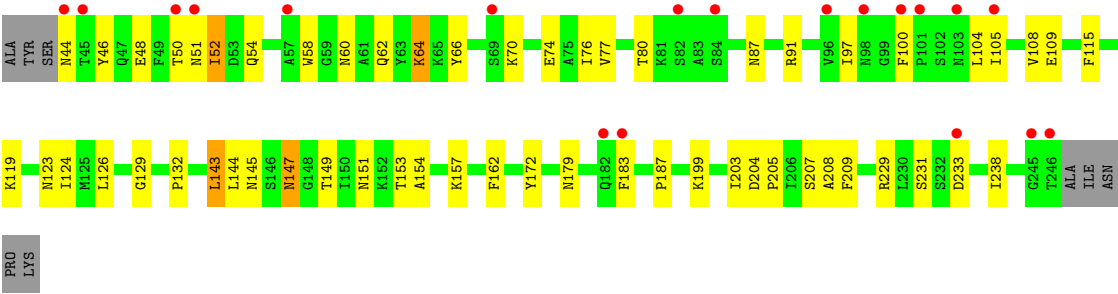


• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3



• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.95Å 74.19Å 119.68Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 25.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-1.95) 91.1 (25.00-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.277 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7223	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, NIR, ADP, 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	0.40	0/1622	0.89	4/2178 (0.2%)
1	B	0.56	2/1688 (0.1%)	1.05	9/2267 (0.4%)
1	C	0.49	0/1664	0.89	4/2234 (0.2%)
1	D	0.41	0/1625	0.92	6/2182 (0.3%)
All	All	0.47	2/6599 (0.0%)	0.94	23/8861 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CD-NE	-10.80	1.31	1.46
1	B	229	ARG	N-CA	5.40	1.52	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	CD-NE-CZ	13.71	143.60	124.40
1	B	229	ARG	NE-CZ-NH1	12.63	134.13	121.50
1	B	229	ARG	NE-CZ-NH2	-12.11	108.30	119.20
1	D	203	ILE	N-CA-C	8.04	120.78	112.83
1	C	203	ILE	N-CA-C	7.73	120.48	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	GLY	N-CA-C	-6.29	106.25	115.30
1	C	66	TYR	N-CA-C	6.20	118.59	111.02
1	B	172	TYR	N-CA-C	-6.15	102.24	110.55
1	A	214	GLU	N-CA-C	6.15	119.18	109.96
1	B	187	PRO	CB-CA-C	-6.13	103.14	111.85
1	D	172	TYR	N-CA-C	-6.00	102.45	110.55
1	B	66	TYR	N-CA-C	5.87	117.37	110.97
1	D	145	ASN	N-CA-C	-5.75	103.12	110.53
1	D	66	TYR	N-CA-C	5.71	117.19	110.97
1	C	172	TYR	N-CA-C	-5.57	103.03	110.55
1	C	52	ILE	N-CA-C	5.49	116.22	110.62
1	A	172	TYR	N-CA-C	-5.42	103.24	110.55
1	A	152	LYS	N-CA-C	5.34	117.10	111.28
1	B	162	PHE	N-CA-C	5.32	120.78	113.97
1	D	162	PHE	N-CA-C	5.25	121.08	114.31
1	A	116	ASN	N-CA-C	-5.11	106.31	112.54
1	D	233	ASP	N-CA-C	-5.11	102.92	110.48
1	B	203	ILE	N-CA-C	5.11	117.02	112.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	229	ARG	Sidechain

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	1594	0	1615	32	0
1	B	1658	0	1677	49	0
1	C	1635	0	1658	30	0
1	D	1597	0	1616	38	0
2	A	44	0	25	0	0
2	B	44	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	C	17	0	16	5	0
5	C	27	0	12	1	0
5	D	27	0	12	0	0
6	A	168	0	0	1	0
6	B	125	0	0	1	0
6	C	139	0	0	4	0
6	D	138	0	0	1	0
All	All	7223	0	6656	148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (148) 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:125:MET:HE3	1:A:191:LYS:HB3	1.40	1.02
1:D:151:ASN:HD22	1:D:154:ALA:H	1.21	0.86
1:B:229:ARG:O	1:B:229:ARG:HG2	1.75	0.85
1:B:66:TYR:HB3	1:B:68:LEU:HD13	1.59	0.85
1:B:188:ILE:HD13	1:B:237:ILE:HB	1.62	0.79
1:B:45:THR:HG23	1:B:123:ASN:HD22	1.49	0.74
1:B:44:ASN:O	1:B:45:THR:HG22	1.89	0.73
1:C:162:PHE:HB3	1:C:225:ILE:HD12	1.73	0.70
1:D:129:GLY:HA3	1:D:183:PHE:HB2	1.72	0.70
1:C:105:ILE:O	1:C:109:GLU:HG3	1.91	0.69
1:D:100:PHE:HD2	1:D:104:LEU:HD22	1.58	0.68
1:B:105:ILE:O	1:B:109:GLU:HG3	1.95	0.66
1:C:152:LYS:O	1:C:156:GLU:HG2	1.95	0.66
1:D:87:ASN:HB3	1:D:91:ARG:HH22	1.63	0.64
1:B:58:TRP:O	1:B:62:GLN:HG2	1.98	0.62
1:A:46:TYR:CD2	1:A:123:ASN:HB3	2.34	0.62
1:B:70:LYS:O	1:B:74:GLU:HG3	2.00	0.62
1:C:147:ASN:OD1	1:C:147:ASN:N	2.30	0.62
1:C:44:ASN:HB3	6:C:2001:HOH:O	1.99	0.62
1:C:87:ASN:O	1:C:91:ARG:HG3	2.02	0.60
1:A:224:HIS:HD2	1:A:226:ASP:OD2	1.84	0.59
1:A:115:PHE:HB3	1:A:199:LYS:HD3	1.84	0.59
1:A:162:PHE:HB3	1:A:225:ILE:HD12	1.84	0.59
1:B:225:ILE:HD13	1:B:239:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:HG2	1:C:139:PHE:CD1	2.38	0.59
1:D:87:ASN:HB3	1:D:91:ARG:NH2	2.18	0.58
1:D:44:ASN:HB2	6:D:2001:HOH:O	2.03	0.58
1:C:155:PHE:CZ	1:C:159:LYS:HE3	2.38	0.58
1:D:46:TYR:CD2	1:D:123:ASN:HB3	2.38	0.58
1:B:66:TYR:HB3	1:B:68:LEU:CD1	2.32	0.57
1:C:83:ALA:HB3	4:C:1252:NIR:H5'3	1.86	0.57
1:C:93:ASN:O	1:C:96:VAL:HG22	2.05	0.57
1:A:125:MET:HE2	1:A:127:PHE:CZ	2.40	0.56
1:B:45:THR:CG2	1:B:123:ASN:HD22	2.17	0.56
1:C:189:ILE:HB	1:C:238:ILE:HD13	1.86	0.56
1:C:132:PRO:HD3	1:C:187:PRO:HG3	1.88	0.55
1:A:87:ASN:HB3	1:A:91:ARG:HH12	1.70	0.55
1:A:162:PHE:HB3	1:A:225:ILE:CD1	2.36	0.55
1:A:164:ASN:HB2	6:A:2108:HOH:O	2.07	0.55
1:B:144:LEU:HD23	1:B:150:ILE:HD13	1.87	0.55
1:B:220:HIS:HD2	1:B:246:THR:O	1.90	0.54
1:D:124:ILE:HD12	1:D:126:LEU:HD21	1.90	0.54
1:D:51:ASN:HD21	1:D:54:GLN:HB2	1.72	0.54
1:D:151:ASN:HD21	1:D:153:THR:HB	1.73	0.54
1:C:183:PHE:CZ	4:C:1252:NIR:H4	2.43	0.54
1:C:93:ASN:HD22	1:C:96:VAL:HG23	1.71	0.53
1:B:144:LEU:CD2	1:B:150:ILE:HD13	2.38	0.53
1:D:97:ILE:HA	1:D:100:PHE:CD1	2.44	0.53
1:D:229:ARG:NH1	1:D:238:ILE:HD12	2.24	0.53
1:A:60:ASN:O	1:A:64:LYS:HG3	2.09	0.52
1:A:124:ILE:HD13	1:A:126:LEU:HD21	1.89	0.52
1:D:119:LYS:HE2	1:D:199:LYS:HG2	1.91	0.52
1:B:156:GLU:HB3	6:B:2070:HOH:O	2.09	0.52
1:A:52:ILE:HD12	1:D:48:GLU:OE2	2.10	0.52
1:B:150:ILE:HG21	1:B:230:LEU:HD21	1.92	0.51
1:A:218:PRO:CG	1:A:246:THR:HG21	2.40	0.51
1:D:153:THR:O	1:D:157:LYS:HG2	2.11	0.51
1:D:76:ILE:O	1:D:80:THR:HG23	2.11	0.51
1:B:102:SER:O	1:B:105:ILE:HG22	2.10	0.51
1:D:115:PHE:HB3	1:D:199:LYS:HD3	1.93	0.51
1:A:79:TYR:CD1	1:A:79:TYR:C	2.90	0.50
1:B:87:ASN:O	1:B:91:ARG:HG3	2.11	0.50
1:B:102:SER:HA	1:B:105:ILE:HG22	1.94	0.50
1:B:111:LEU:HD23	1:B:172:TYR:CZ	2.46	0.49
2:B:1252:NAD:O5D	2:B:1252:NAD:C1D	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:ND2	1:C:96:VAL:HG23	2.27	0.49
1:A:125:MET:HE1	1:A:191:LYS:HD2	1.93	0.49
1:D:179:ASN:HA	1:D:183:PHE:HE1	1.76	0.49
1:B:62:GLN:HE22	1:B:65:LYS:NZ	2.11	0.49
1:B:114:SER:OG	1:B:118:MET:HE2	2.12	0.49
1:B:163:LEU:HD21	1:C:163:LEU:HD21	1.94	0.49
1:B:189:ILE:HD13	1:B:236:GLN:NE2	2.27	0.49
1:C:47:GLN:HE21	1:C:47:GLN:HA	1.76	0.49
1:B:97:ILE:HG22	1:B:100:PHE:HE2	1.77	0.49
1:B:89:LYS:HE3	1:B:100:PHE:CD1	2.49	0.48
4:C:1252:NIR:H5'1	5:C:1253:ADP:O1B	2.14	0.48
1:C:52:ILE:HD13	1:C:178:MET:SD	2.54	0.48
1:B:104:LEU:HD23	1:B:104:LEU:O	2.13	0.48
1:B:204:ASP:HB2	1:B:205:PRO:HD3	1.95	0.48
1:C:124:ILE:HD12	1:C:126:LEU:HD21	1.96	0.48
1:B:135:LEU:HD11	1:B:188:ILE:HD11	1.96	0.48
1:B:51:ASN:HD21	1:B:53:ASP:HB2	1.79	0.48
1:D:229:ARG:HH12	1:D:238:ILE:HD12	1.79	0.48
1:D:87:ASN:CB	1:D:91:ARG:HH22	2.26	0.48
1:D:132:PRO:HD3	1:D:187:PRO:HG3	1.96	0.48
1:B:89:LYS:HE3	1:B:100:PHE:CE1	2.49	0.47
1:D:64:LYS:HZ3	1:D:64:LYS:HA	1.80	0.47
1:B:188:ILE:C	1:B:189:ILE:HD12	2.39	0.47
1:C:231:SER:O	1:C:232:SER:C	2.58	0.47
1:B:97:ILE:HG22	1:B:100:PHE:CE2	2.49	0.47
1:D:105:ILE:O	1:D:109:GLU:HG3	2.15	0.47
1:B:210:ALA:HB1	1:B:214:GLU:OE2	2.14	0.46
1:A:212:GLN:O	1:A:213:LEU:C	2.59	0.46
1:B:104:LEU:O	1:B:108:VAL:HG23	2.15	0.46
1:C:69:SER:OG	1:C:72:GLU:HG3	2.14	0.46
1:B:150:ILE:HG21	1:B:230:LEU:CD2	2.44	0.46
1:C:97:ILE:HB	1:C:105:ILE:HG12	1.97	0.46
1:D:147:ASN:HD22	1:D:147:ASN:C	2.24	0.46
1:D:70:LYS:HG2	1:D:74:GLU:OE2	2.16	0.46
1:B:104:LEU:HD23	1:B:104:LEU:C	2.41	0.45
1:A:69:SER:OG	1:A:72:GLU:HG3	2.16	0.45
1:B:144:LEU:HD23	1:B:150:ILE:HA	1.97	0.45
1:B:188:ILE:O	1:B:189:ILE:HD12	2.17	0.45
1:C:79:TYR:HB2	1:C:111:LEU:HD11	1.99	0.45
1:A:132:PRO:HD3	1:A:187:PRO:HG3	1.98	0.45
1:D:204:ASP:HB2	1:D:205:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:THR:OG1	1:D:209:PHE:HB2	2.17	0.45
1:D:147:ASN:ND2	1:D:149:THR:H	2.15	0.45
1:C:132:PRO:HG3	1:C:143:LEU:HD23	1.98	0.45
1:B:186:ARG:HB3	1:B:187:PRO:HD2	1.98	0.45
1:A:145:ASN:HB2	1:A:149:THR:O	2.17	0.44
1:B:102:SER:C	1:B:105:ILE:HG22	2.42	0.44
1:D:60:ASN:O	1:D:64:LYS:HG2	2.17	0.44
1:C:175:THR:O	4:C:1252:NIR:H5N	2.18	0.44
1:A:217:LEU:HD13	1:A:243:MET:HE3	2.00	0.44
1:D:104:LEU:HD23	1:D:108:VAL:HG23	1.99	0.43
1:D:143:LEU:HB3	1:D:144:LEU:HD12	2.00	0.43
1:D:58:TRP:O	1:D:62:GLN:HG2	2.19	0.43
1:A:204:ASP:HB3	1:A:205:PRO:HD3	2.00	0.42
1:B:165:LYS:HE2	1:C:164:ASN:ND2	2.34	0.42
1:D:52:ILE:H	1:D:52:ILE:HG13	1.47	0.42
1:A:125:MET:CE	1:A:191:LYS:HB3	2.30	0.42
1:A:218:PRO:HG2	1:A:246:THR:CG2	2.49	0.42
1:A:220:HIS:O	1:A:246:THR:HA	2.20	0.42
1:A:124:ILE:HG12	1:A:125:MET:N	2.35	0.42
1:B:204:ASP:N	1:B:205:PRO:CD	2.82	0.42
1:D:64:LYS:HA	1:D:64:LYS:NZ	2.34	0.42
1:B:103:ASN:O	1:B:107:GLN:HG3	2.20	0.41
1:C:139:PHE:HA	1:C:142:THR:OG1	2.20	0.41
1:B:157:LYS:HE3	1:D:208:ALA:O	2.20	0.41
1:A:76:ILE:O	1:A:80:THR:HG23	2.20	0.41
1:B:139:PHE:HA	1:B:142:THR:OG1	2.20	0.41
1:A:58:TRP:O	1:A:62:GLN:HG2	2.21	0.41
1:A:179:ASN:OD1	1:A:184:ALA:HB2	2.20	0.41
1:A:170:TYR:O	1:A:219:ARG:HB2	2.21	0.41
1:D:151:ASN:ND2	1:D:153:THR:HB	2.35	0.41
1:B:188:ILE:HD11	1:B:237:ILE:HD12	2.02	0.41
1:A:202:TYR:CZ	1:A:204:ASP:HB3	2.56	0.41
1:B:225:ILE:HD13	1:B:239:ILE:CG2	2.50	0.41
1:D:77:VAL:HG22	1:D:207:SER:HB2	2.02	0.40
1:D:204:ASP:N	1:D:205:PRO:CD	2.84	0.40
1:C:220:HIS:HD2	6:C:2134:HOH:O	2.04	0.40
4:C:1252:NIR:H3'	6:C:2033:HOH:O	2.21	0.40
1:A:179:ASN:OD1	1:A:184:ALA:CB	2.69	0.40
1:A:202:TYR:CE2	1:A:204:ASP:HB3	2.57	0.40
1:B:62:GLN:HE22	1:B:65:LYS:HZ2	1.68	0.40
1:C:46:TYR:CD2	1:C:123:ASN:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:HG12	6:C:2007:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/211 (95%)	195 (97%)	6 (3%)	0	100	100
1	B	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
1	C	206/211 (98%)	199 (97%)	6 (3%)	1 (0%)	24	16
1	D	201/211 (95%)	198 (98%)	3 (2%)	0	100	100
All	All	817/844 (97%)	794 (97%)	22 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	146	SER

5.3.2 Protein sidechains [i](#)

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	172/179 (96%)	170 (99%)	2 (1%)	63	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	179/179 (100%)	170 (95%)	9 (5%)	22	11
1	C	177/179 (99%)	172 (97%)	5 (3%)	38	30
1	D	173/179 (97%)	167 (96%)	6 (4%)	32	22
All	All	701/716 (98%)	679 (97%)	22 (3%)	35	26

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	124	ILE
1	B	45	THR
1	B	54	GLN
1	B	85	GLU
1	B	97	ILE
1	B	143	LEU
1	B	159	LYS
1	B	225	ILE
1	B	229	ARG
1	B	236	GLN
1	C	47	GLN
1	C	64	LYS
1	C	93	ASN
1	C	140	GLN
1	C	147	ASN
1	D	50	THR
1	D	52	ILE
1	D	64	LYS
1	D	143	LEU
1	D	147	ASN
1	D	231	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	60	ASN
1	A	62	GLN
1	A	92	GLN
1	A	107	GLN
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	140	GLN
1	A	141	ASN
1	A	182	GLN
1	A	212	GLN
1	B	44	ASN
1	B	51	ASN
1	B	54	GLN
1	B	60	ASN
1	B	62	GLN
1	B	103	ASN
1	B	141	ASN
1	B	147	ASN
1	B	182	GLN
1	B	220	HIS
1	B	236	GLN
1	C	44	ASN
1	C	47	GLN
1	C	92	GLN
1	C	93	ASN
1	C	107	GLN
1	C	141	ASN
1	C	151	ASN
1	C	182	GLN
1	C	212	GLN
1	C	249	ASN
1	D	51	ASN
1	D	54	GLN
1	D	60	ASN
1	D	92	GLN
1	D	116	ASN
1	D	140	GLN
1	D	145	ASN
1	D	147	ASN
1	D	151	ASN
1	D	182	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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$
5	ADP	D	1247	-	28,29,29	2.16	10 (35%)	43,45,45	2.41	17 (39%)
4	NIR	C	1252	-	17,18,18	4.08	7 (41%)	20,26,26	3.70	8 (40%)
2	NAD	B	1252	-	46,48,48	1.14	5 (10%)	64,73,73	2.36	17 (26%)
3	SO4	B	1253	-	4,4,4	2.30	2 (50%)	6,6,6	0.17	0
5	ADP	C	1253	-	28,29,29	1.04	1 (3%)	43,45,45	1.24	3 (6%)
3	SO4	A	1249	-	4,4,4	2.33	2 (50%)	6,6,6	0.14	0
2	NAD	A	1248	-	46,48,48	2.60	12 (26%)	64,73,73	2.13	23 (35%)

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
5	ADP	D	1247	-	-	3/16/32/32	0/3/3/3
2	NAD	A	1248	-	1/1/11/11	5/30/62/62	0/5/5/5
4	NIR	C	1252	-	2/2/7/9	4/8/34/34	0/2/2/2
2	NAD	B	1252	-	1/1/11/11	8/30/62/62	0/5/5/5
5	ADP	C	1253	-	-	3/16/32/32	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1252	NIR	C4-C5	-12.01	1.38	1.53
2	A	1248	NAD	PN-O3	-7.94	1.50	1.59
2	A	1248	NAD	PA-O3	7.70	1.67	1.59
2	A	1248	NAD	O4D-C1D	-7.16	1.31	1.40
4	C	1252	NIR	C4-N9	-6.32	1.37	1.47
4	C	1252	NIR	C8-C5N	-5.94	1.34	1.49
2	A	1248	NAD	C3N-C7N	5.90	1.59	1.50
5	D	1247	ADP	C2'-C1'	-5.14	1.37	1.53
5	D	1247	ADP	C2-N1	4.97	1.42	1.33
4	C	1252	NIR	C5-C4N	-4.90	1.41	1.52
2	A	1248	NAD	C2N-N1N	4.62	1.40	1.35
2	A	1248	NAD	C2A-N1A	4.15	1.41	1.33
4	C	1252	NIR	C4N-C5N	3.57	1.41	1.32
5	D	1247	ADP	O4'-C4'	-3.40	1.37	1.45
5	D	1247	ADP	C5-C4	-3.36	1.33	1.39
5	D	1247	ADP	PB-O2B	-3.34	1.42	1.54
5	D	1247	ADP	PA-O2A	-3.24	1.40	1.55
4	C	1252	NIR	C8-N9	-3.21	1.39	1.47
2	B	1252	NAD	PN-O3	3.12	1.62	1.59
3	A	1249	SO4	O1-S	2.90	1.62	1.44
3	B	1253	SO4	O2-S	2.88	1.61	1.44
3	A	1249	SO4	O2-S	2.86	1.61	1.44
2	B	1252	NAD	C6N-N1N	2.80	1.41	1.35
3	B	1253	SO4	O1-S	2.75	1.61	1.44
5	D	1247	ADP	C3'-C4'	-2.73	1.46	1.53
2	A	1248	NAD	PN-O1N	-2.69	1.41	1.50
5	D	1247	ADP	PB-O1B	2.60	1.58	1.50
5	C	1253	ADP	PB-O3B	-2.58	1.45	1.54
2	B	1252	NAD	C3N-C7N	2.48	1.54	1.50
4	C	1252	NIR	C2'-C1'	-2.46	1.45	1.53
2	A	1248	NAD	C6N-N1N	2.42	1.40	1.35
2	A	1248	NAD	C5B-C4B	2.36	1.58	1.51
2	B	1252	NAD	C2A-N1A	2.35	1.38	1.33
2	A	1248	NAD	C5A-C4A	-2.29	1.35	1.39
5	D	1247	ADP	C5-N7	-2.28	1.34	1.39
2	A	1248	NAD	C7N-N7N	2.19	1.37	1.33
2	B	1252	NAD	C2N-N1N	2.17	1.37	1.35
2	A	1248	NAD	C5A-N7A	-2.04	1.35	1.39
5	D	1247	ADP	PA-O5'	2.02	1.67	1.59

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1252	NIR	C4-C5-C4N	8.48	120.74	108.63
4	C	1252	NIR	C8-N9-C4	7.55	121.06	109.43
2	B	1252	NAD	C5N-C4N-C3N	-7.44	113.05	120.36
2	B	1252	NAD	O7N-C7N-C3N	7.20	128.40	119.60
2	B	1252	NAD	C4D-O4D-C1D	-6.97	103.55	109.92
2	B	1252	NAD	C6N-C5N-C4N	6.39	128.66	119.45
4	C	1252	NIR	C5'-C4'-C3'	6.33	122.34	115.70
5	D	1247	ADP	O2B-PB-O3A	6.29	125.73	104.64
4	C	1252	NIR	C5-C4N-C5N	-6.12	112.91	123.33
5	D	1247	ADP	O3B-PB-O1B	-5.64	88.87	110.83
4	C	1252	NIR	C8-N9-C1'	5.04	127.54	112.93
2	B	1252	NAD	C5N-C6N-N1N	-5.01	113.55	120.38
5	D	1247	ADP	O5'-PA-O1A	-4.97	89.25	108.94
2	A	1248	NAD	O2A-PA-O5B	4.84	129.50	107.57
2	A	1248	NAD	N6A-C6A-N1A	4.66	128.76	118.38
5	D	1247	ADP	N6-C6-N1	4.40	128.18	118.38
2	A	1248	NAD	O2N-PN-O3	4.21	118.65	107.27
2	B	1252	NAD	O7N-C7N-N7N	-4.07	116.74	122.62
5	D	1247	ADP	O2A-PA-O1A	4.07	131.36	112.44
2	A	1248	NAD	O3-PN-O1N	3.78	122.07	110.70
2	A	1248	NAD	O7N-C7N-N7N	3.74	128.02	122.62
5	D	1247	ADP	O2A-PA-O5'	3.66	124.14	107.57
5	C	1253	ADP	O3B-PB-O3A	3.54	116.50	104.64
5	D	1247	ADP	C6-C5-C4	3.49	121.95	117.18
5	D	1247	ADP	N9-C8-N7	-3.49	108.98	113.94
2	A	1248	NAD	C5N-C6N-N1N	-3.46	115.66	120.38
2	A	1248	NAD	C4D-O4D-C1D	-3.41	106.80	109.92
2	A	1248	NAD	O2N-PN-O5D	-3.32	92.53	107.57
2	A	1248	NAD	C6A-C5A-C4A	3.20	121.55	117.18
2	B	1252	NAD	N6A-C6A-N1A	3.20	125.50	118.38
2	A	1248	NAD	C5A-C6A-N6A	-3.16	115.46	123.29
2	A	1248	NAD	C2D-C3D-C4D	-3.14	96.55	102.61
2	A	1248	NAD	C3N-C7N-N7N	-3.13	113.88	117.74
5	C	1253	ADP	O3A-PA-O1A	3.12	120.08	110.70
2	A	1248	NAD	C6A-C5A-N7A	-3.11	126.09	132.09
5	D	1247	ADP	C6-C5-N7	-3.04	126.22	132.09
2	B	1252	NAD	O2A-PA-O3	2.97	115.29	107.27
2	A	1248	NAD	O5D-PN-O1N	-2.97	97.18	108.94
4	C	1252	NIR	C8-C5N-C4N	2.96	129.01	123.06
2	B	1252	NAD	C2N-C3N-C4N	2.92	121.65	118.26
2	A	1248	NAD	O2B-C2B-C1B	2.82	119.81	110.10
2	A	1248	NAD	C5D-C4D-C3D	-2.79	105.16	115.21
2	B	1252	NAD	O5D-PN-O1N	2.75	119.85	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1247	ADP	C5-C6-N6	-2.74	116.50	123.29
4	C	1252	NIR	C4N-C5-C6	2.71	117.41	109.80
2	B	1252	NAD	O2A-PA-O1A	-2.69	99.95	112.44
2	A	1248	NAD	N3A-C2A-N1A	2.68	132.64	128.58
5	C	1253	ADP	O2A-PA-O3A	2.65	114.43	107.27
5	D	1247	ADP	C2'-C3'-C4'	2.65	107.72	102.61
5	D	1247	ADP	O3B-PB-O3A	2.63	113.45	104.64
2	B	1252	NAD	O2B-C2B-C1B	2.51	118.76	110.10
5	D	1247	ADP	O3'-C3'-C4'	2.51	118.28	111.08
2	A	1248	NAD	N9A-C8A-N7A	-2.50	110.39	113.94
2	B	1252	NAD	C6N-N1N-C1D	2.47	124.58	119.73
2	A	1248	NAD	O4B-C1B-N9A	2.46	112.81	108.09
2	B	1252	NAD	C2N-N1N-C1D	-2.37	113.91	119.13
5	D	1247	ADP	O2B-PB-O1B	-2.35	101.66	110.83
2	B	1252	NAD	C3N-C7N-N7N	-2.34	114.85	117.74
2	A	1248	NAD	C2A-N3A-C4A	-2.27	106.28	111.83
5	D	1247	ADP	O4'-C4'-C3'	-2.25	100.69	105.15
4	C	1252	NIR	O3'-C3'-C4'	-2.23	105.01	110.47
5	D	1247	ADP	C3'-C2'-C1'	-2.23	97.25	101.46
2	A	1248	NAD	O4D-C4D-C5D	-2.22	102.23	109.33
2	A	1248	NAD	O3B-C3B-C4B	2.18	117.35	111.08
2	B	1252	NAD	O2A-PA-O5B	2.17	117.42	107.57
5	D	1247	ADP	O2'-C2'-C1'	2.17	117.59	110.10
2	A	1248	NAD	C4N-C3N-C7N	-2.15	115.21	121.06
2	B	1252	NAD	C2A-N1A-C6A	2.01	122.04	118.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1248	NAD	C1D
2	B	1252	NAD	C1D
4	C	1252	NIR	C5
4	C	1252	NIR	C1'

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1252	NAD	C2D-C1D-N1N-C2N
4	C	1252	NIR	C2'-C1'-N9-C8
4	C	1252	NIR	O4'-C1'-N9-C8
2	B	1252	NAD	O4D-C4D-C5D-O5D
2	A	1248	NAD	O4D-C4D-C5D-O5D

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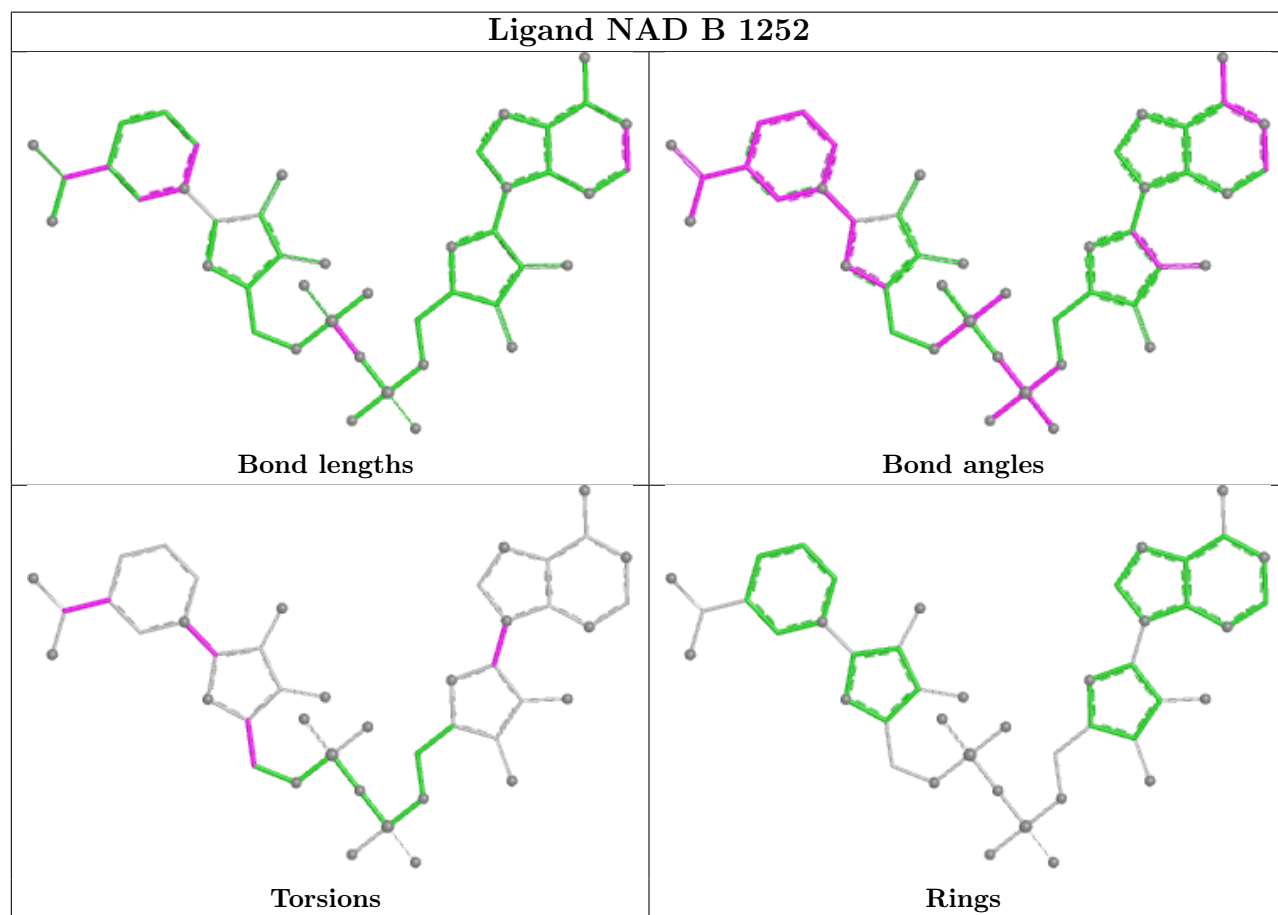
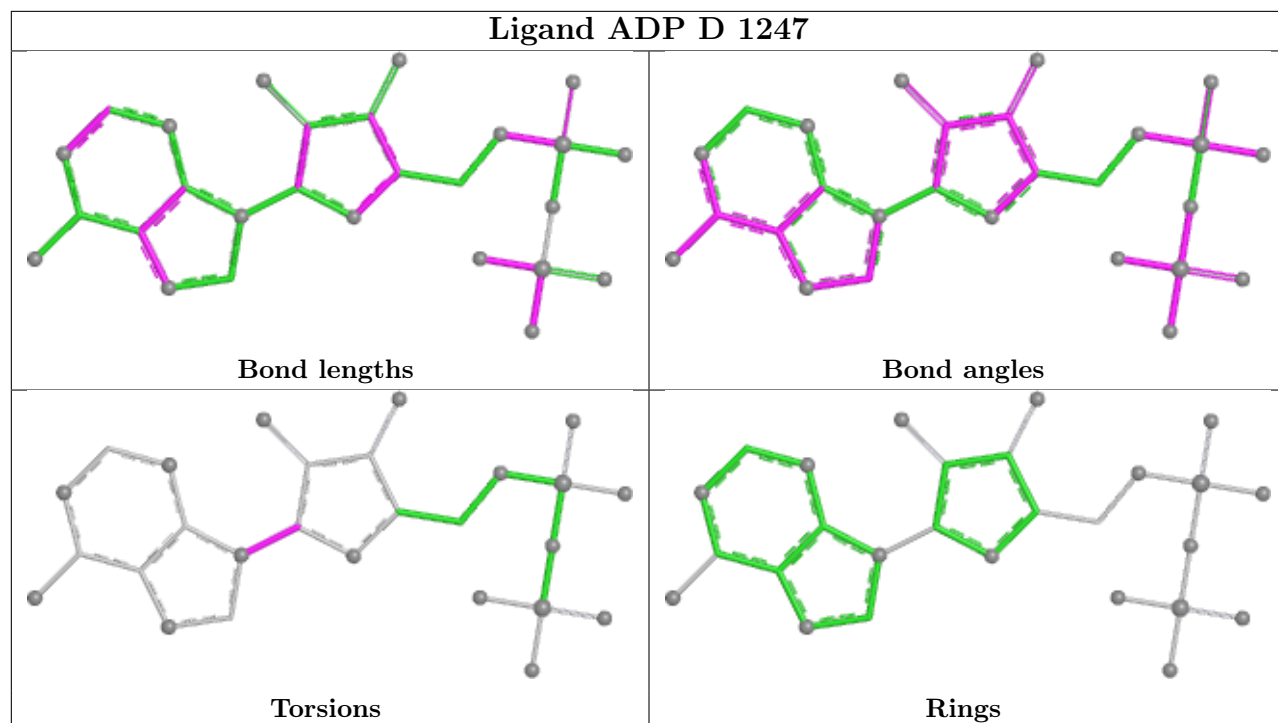
Mol	Chain	Res	Type	Atoms
4	C	1252	NIR	C4-C5-C6-N1
2	A	1248	NAD	C3D-C4D-C5D-O5D
5	C	1253	ADP	C2'-C1'-N9-C8
2	A	1248	NAD	C2B-C1B-N9A-C8A
2	B	1252	NAD	C2B-C1B-N9A-C8A
5	D	1247	ADP	C2'-C1'-N9-C8
4	C	1252	NIR	C4-C5-C6-O6
2	A	1248	NAD	C2B-C1B-N9A-C4A
5	C	1253	ADP	C2'-C1'-N9-C4
5	D	1247	ADP	C2'-C1'-N9-C4
2	B	1252	NAD	C2D-C1D-N1N-C6N
2	B	1252	NAD	C4N-C3N-C7N-O7N
2	B	1252	NAD	C4N-C3N-C7N-N7N
2	B	1252	NAD	C3D-C4D-C5D-O5D
2	B	1252	NAD	O4B-C1B-N9A-C8A
5	C	1253	ADP	O4'-C1'-N9-C8
5	D	1247	ADP	O4'-C1'-N9-C8
2	A	1248	NAD	O4B-C1B-N9A-C8A

There are no ring outliers.

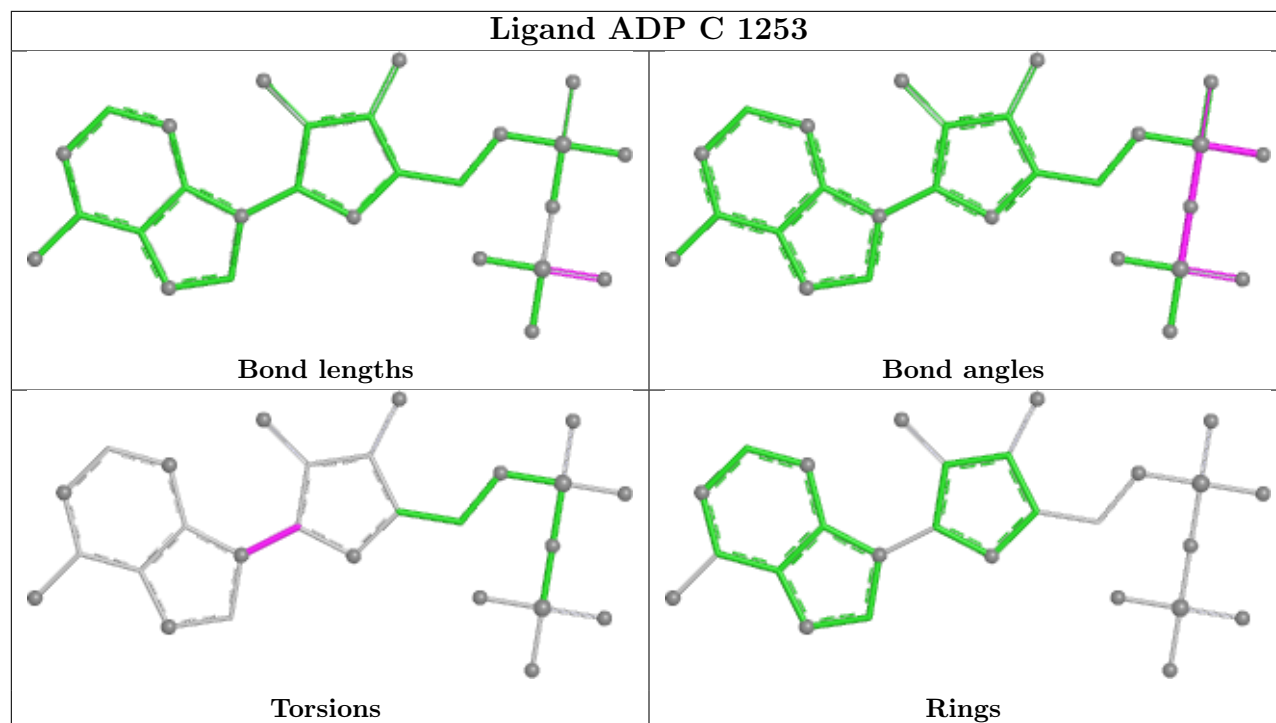
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1252	NIR	5	0
2	B	1252	NAD	1	0
5	C	1253	ADP	1	0

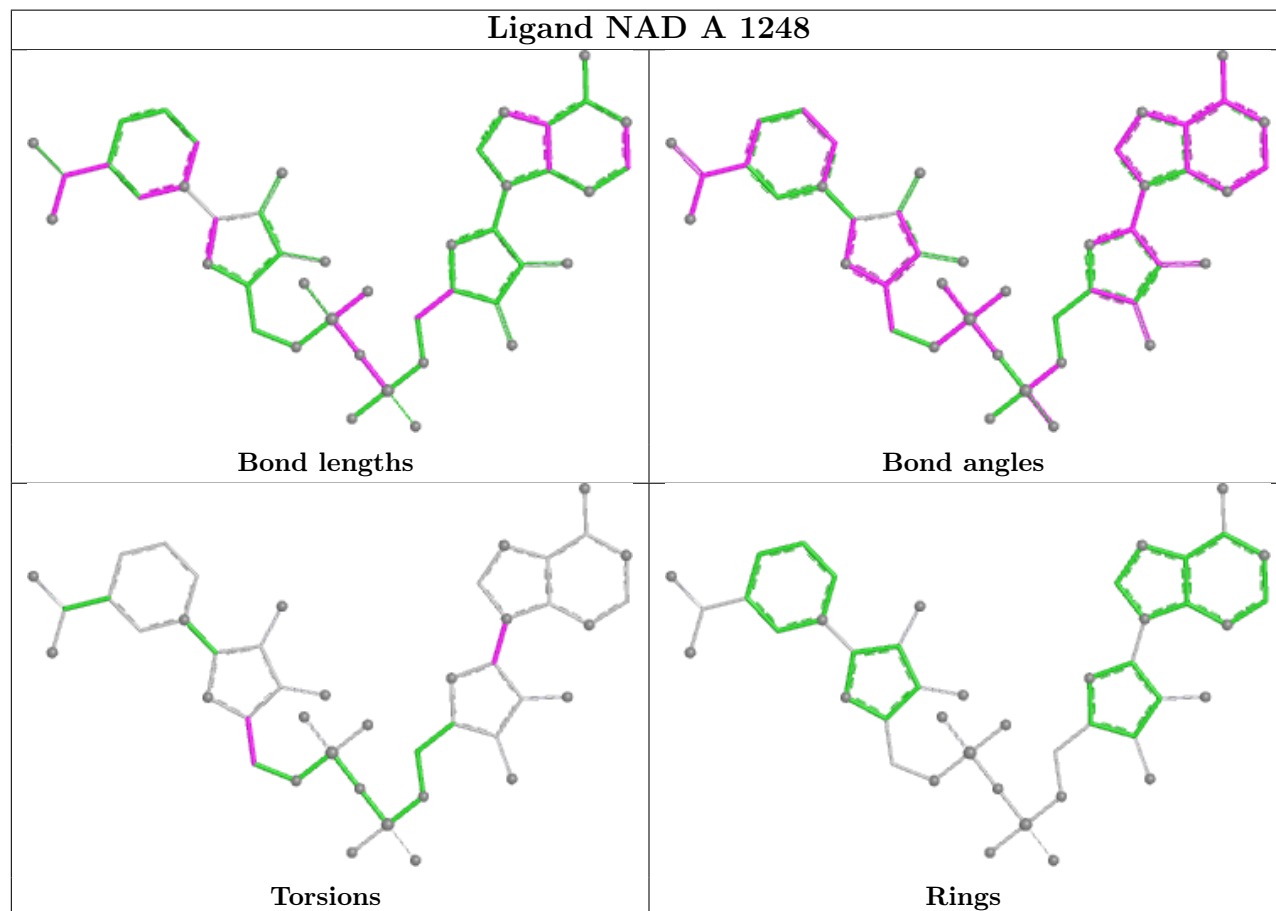
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand ADP C 1253



Ligand NAD A 1248



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	203/211 (96%)	0.50	9 (4%) 39 45	24, 33, 43, 77	0
1	B	211/211 (100%)	0.97	38 (18%) 3 3	24, 38, 58, 67	0
1	C	208/211 (98%)	0.68	21 (10%) 12 14	20, 34, 57, 64	0
1	D	203/211 (96%)	0.72	19 (9%) 14 16	22, 35, 56, 71	0
All	All	825/844 (97%)	0.72	87 (10%) 11 13	20, 35, 57, 77	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	ASN	5.2
1	C	149	THR	4.9
1	B	183	PHE	4.6
1	B	102	SER	4.1
1	A	247	ALA	4.0
1	A	146	SER	4.0
1	A	244	MET	3.9
1	C	97	ILE	3.8
1	A	245	GLY	3.7
1	D	246	THR	3.6
1	B	100	PHE	3.4
1	B	44	ASN	3.3
1	C	96	VAL	3.3
1	B	230	LEU	3.3
1	D	105	ILE	3.2
1	C	103	ASN	3.2
1	B	229	ARG	3.2
1	B	105	ILE	3.1
1	D	183	PHE	3.1
1	B	97	ILE	3.0
1	D	96	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	245	GLY	3.0
1	B	99	GLY	2.9
1	B	150	ILE	2.9
1	B	154	ALA	2.9
1	C	234	GLY	2.9
1	B	95	GLY	2.9
1	C	99	GLY	2.9
1	B	71	SER	2.8
1	C	98	ASN	2.8
1	C	145	ASN	2.8
1	B	45	THR	2.8
1	B	85	GLU	2.8
1	A	54	GLN	2.7
1	B	98	ASN	2.7
1	D	100	PHE	2.7
1	C	146	SER	2.7
1	D	233	ASP	2.7
1	A	246	THR	2.6
1	B	185	GLY	2.6
1	B	96	VAL	2.6
1	B	103	ASN	2.6
1	B	147	ASN	2.6
1	C	231	SER	2.6
1	B	234	GLY	2.6
1	B	232	SER	2.6
1	B	149	THR	2.6
1	B	101	PRO	2.5
1	C	148	GLY	2.5
1	B	181	SER	2.5
1	D	57	ALA	2.5
1	B	153	THR	2.5
1	C	140	GLN	2.5
1	B	143	LEU	2.5
1	B	184	ALA	2.5
1	B	83	ALA	2.4
1	C	44	ASN	2.4
1	D	98	ASN	2.4
1	D	103	ASN	2.4
1	B	146	SER	2.4
1	B	231	SER	2.4
1	B	155	PHE	2.4
1	B	51	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	95	GLY	2.3
1	D	44	ASN	2.3
1	D	45	THR	2.3
1	C	227	ASP	2.2
1	C	141	ASN	2.2
1	B	144	LEU	2.2
1	B	84	SER	2.2
1	D	82	SER	2.2
1	D	101	PRO	2.2
1	C	154	ALA	2.2
1	A	45	THR	2.2
1	C	238	ILE	2.2
1	D	51	ASN	2.1
1	C	100	PHE	2.1
1	D	50	THR	2.1
1	D	69	SER	2.1
1	B	41	ALA	2.1
1	A	105	ILE	2.1
1	B	188	ILE	2.1
1	B	180	VAL	2.1
1	D	84	SER	2.0
1	C	153	THR	2.0
1	C	156	GLU	2.0
1	D	182	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

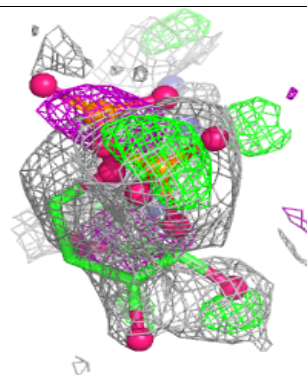
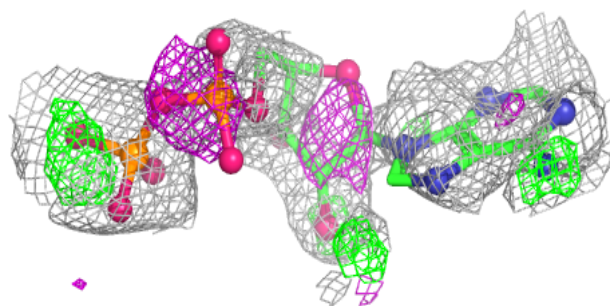
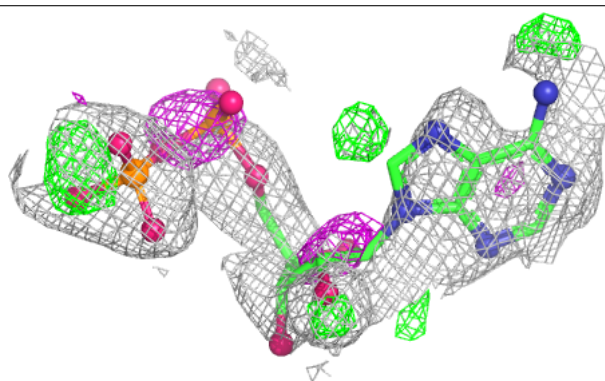
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ADP	D	1247	27/27	0.53	0.20	78,80,86,86	0
4	NIR	C	1252	17/17	0.75	0.16	45,53,70,73	0
5	ADP	C	1253	27/27	0.83	0.15	72,77,84,85	0
2	NAD	B	1252	44/44	0.86	0.13	37,53,71,72	0
3	SO4	B	1253	5/5	0.91	0.12	51,52,54,54	0
3	SO4	A	1249	5/5	0.92	0.10	51,52,55,55	0
2	NAD	A	1248	44/44	0.93	0.09	23,33,40,43	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.

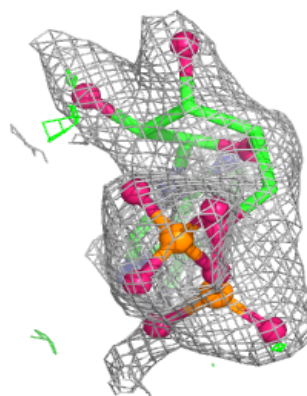
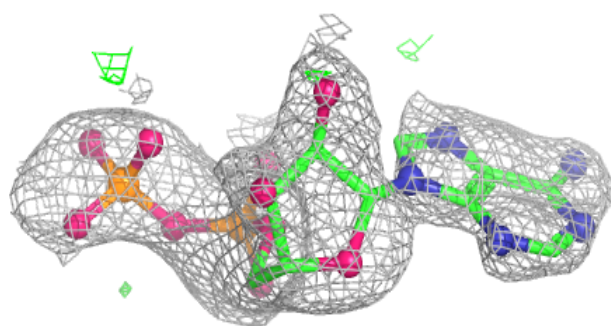
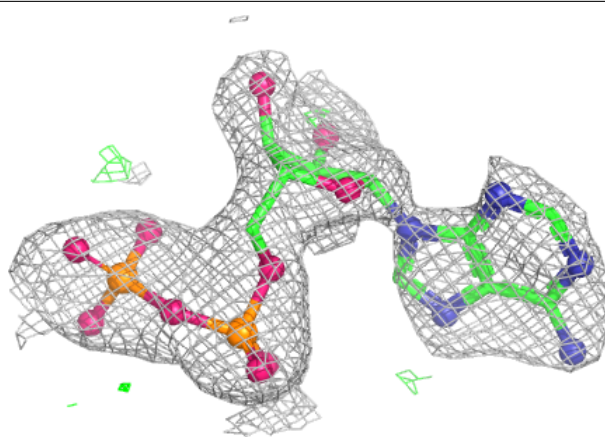
Electron density around ADP D 1247:

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

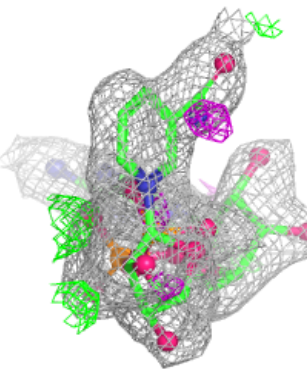
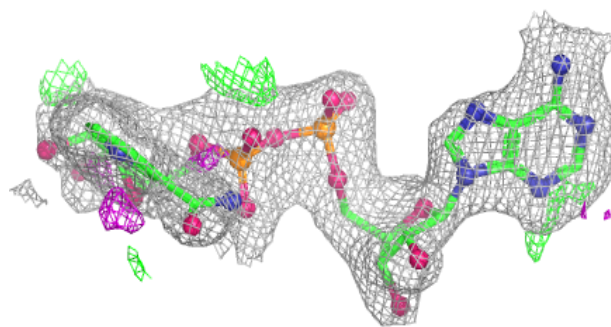
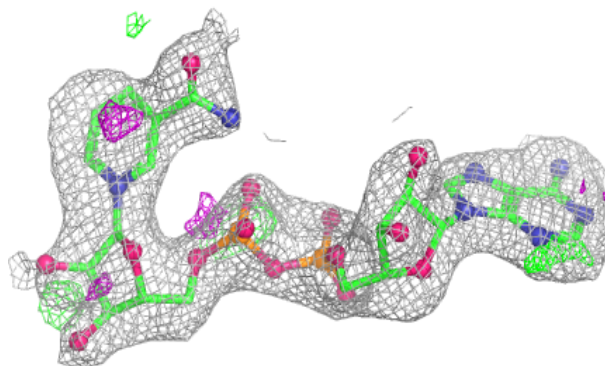


Electron density around ADP C 1253:

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

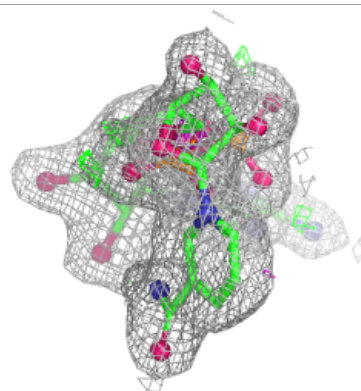
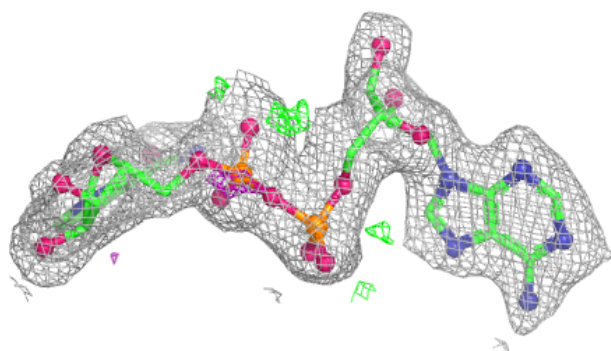
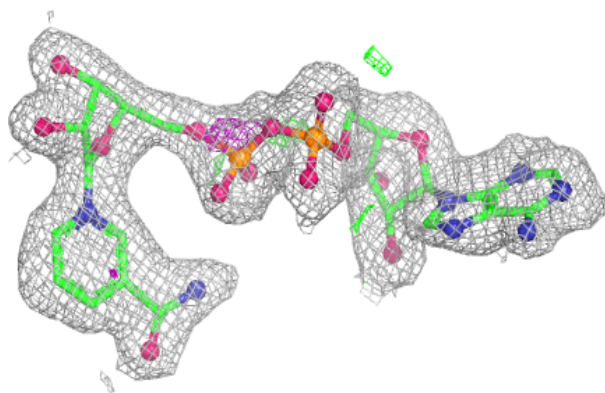
**Electron density around NAD B 1252:**

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



Electron density around NAD A 1248:

$2mF_o-DF_c$ (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.