



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:18 am BST

PDB ID : 3Q6I
Title : Crystal structure of FabG4 and coenzyme binary complex
Authors : Dutta, D.; Bhattacharyya, S.; Das, A.K.
Deposited on : 2011-01-01
Resolution : 2.59 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

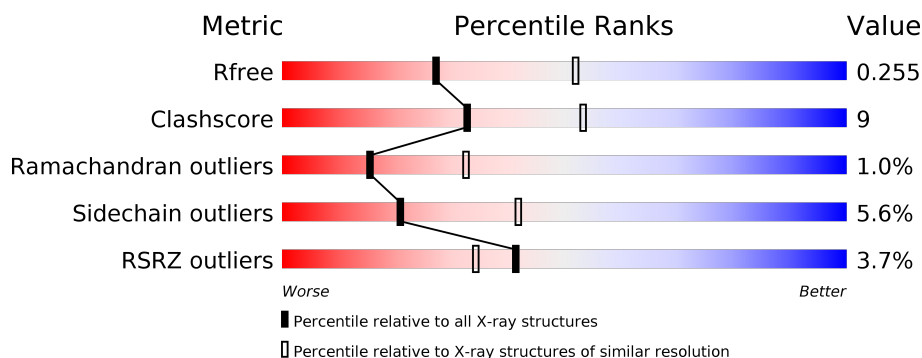
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	446	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 17%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% 76% 17% 6% </div> </div>
1	B	446	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 77%, yellow 18%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% 77% 18% 5% </div> </div>
1	C	446	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 74%, yellow 17%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% 74% 17% 6% </div> </div>
1	D	446	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, green 69%, yellow 21%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% 69% 21% 8% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12462 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 3-oxoacyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3080	1925	553	595	7			
1	B	425	Total	C	N	O	S	0	0	0
			3059	1916	543	593	7			
1	C	418	Total	C	N	O	S	0	0	0
			2991	1871	530	584	6			
1	D	409	Total	C	N	O	S	0	0	0
			2927	1836	514	571	6			

There are 32 discrepancies between the modelled and reference sequences:

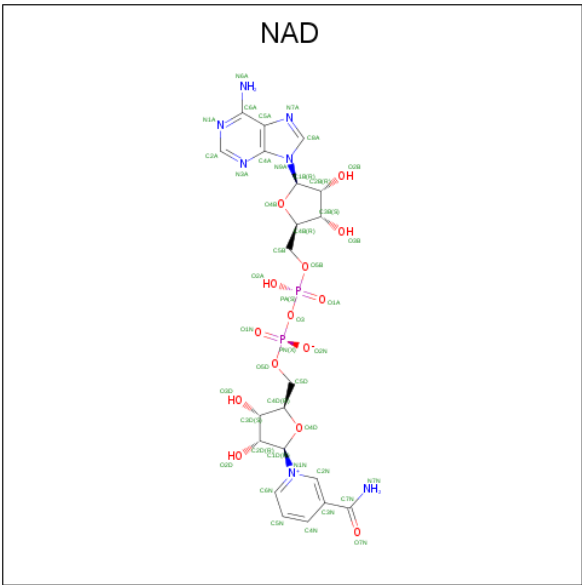
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	HIS	-	EXPRESSION TAG	UNP O53665
A	10	HIS	-	EXPRESSION TAG	UNP O53665
A	11	HIS	-	EXPRESSION TAG	UNP O53665
A	12	HIS	-	EXPRESSION TAG	UNP O53665
A	13	HIS	-	EXPRESSION TAG	UNP O53665
A	14	HIS	-	EXPRESSION TAG	UNP O53665
A	15	GLY	-	EXPRESSION TAG	UNP O53665
A	16	SER	-	EXPRESSION TAG	UNP O53665
B	9	HIS	-	EXPRESSION TAG	UNP O53665
B	10	HIS	-	EXPRESSION TAG	UNP O53665
B	11	HIS	-	EXPRESSION TAG	UNP O53665
B	12	HIS	-	EXPRESSION TAG	UNP O53665
B	13	HIS	-	EXPRESSION TAG	UNP O53665
B	14	HIS	-	EXPRESSION TAG	UNP O53665
B	15	GLY	-	EXPRESSION TAG	UNP O53665
B	16	SER	-	EXPRESSION TAG	UNP O53665
C	9	HIS	-	EXPRESSION TAG	UNP O53665
C	10	HIS	-	EXPRESSION TAG	UNP O53665
C	11	HIS	-	EXPRESSION TAG	UNP O53665
C	12	HIS	-	EXPRESSION TAG	UNP O53665
C	13	HIS	-	EXPRESSION TAG	UNP O53665

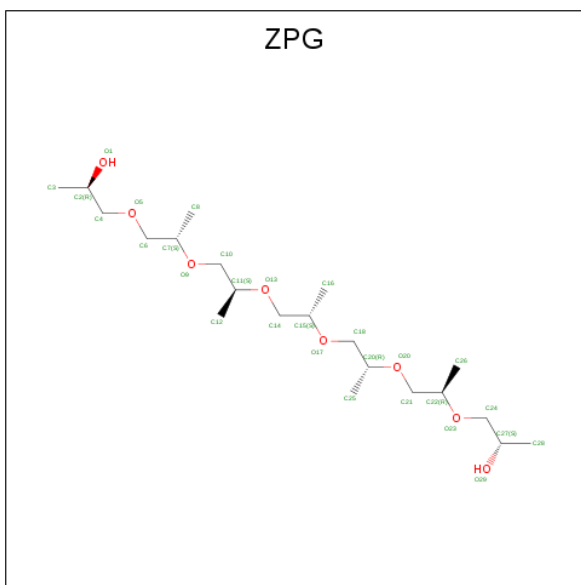
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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	HIS	-	EXPRESSION TAG	UNP O53665
C	15	GLY	-	EXPRESSION TAG	UNP O53665
C	16	SER	-	EXPRESSION TAG	UNP O53665
D	9	HIS	-	EXPRESSION TAG	UNP O53665
D	10	HIS	-	EXPRESSION TAG	UNP O53665
D	11	HIS	-	EXPRESSION TAG	UNP O53665
D	12	HIS	-	EXPRESSION TAG	UNP O53665
D	13	HIS	-	EXPRESSION TAG	UNP O53665
D	14	HIS	-	EXPRESSION TAG	UNP O53665
D	15	GLY	-	EXPRESSION TAG	UNP O53665
D	16	SER	-	EXPRESSION TAG	UNP O53665

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).





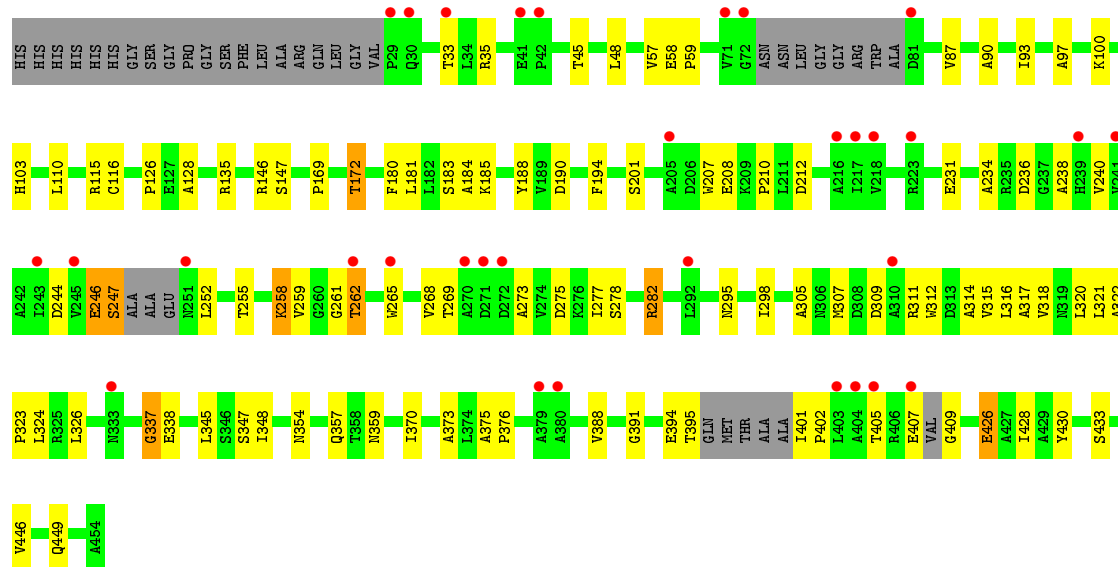
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	69	Total O 69 69	0	0
4	C	39	Total O 39 39	0	0
4	D	30	Total O 30 30	0	0



- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.07Å 71.03Å 92.92Å 105.02° 97.06° 93.66°	Depositor
Resolution (Å)	19.78 – 2.59 19.78 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.78-2.59) 95.7 (19.78-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.168 , 0.242 0.194 , 0.255	Depositor DCC
R_{free} test set	2322 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12462	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.70	0/3125	0.83	1/4248 (0.0%)
1	B	0.70	0/3102	0.77	1/4212 (0.0%)
1	C	0.65	0/3036	0.76	0/4132
1	D	0.61	0/2968	0.73	0/4032
All	All	0.67	0/12231	0.77	2/16624 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	LEU	CA-CB-CG	-6.02	101.45	115.30
1	B	345	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3080	0	3100	63	0
1	B	3059	0	3073	55	0
1	C	2991	0	2963	51	0
1	D	2927	0	2916	56	0
2	A	44	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	3	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	13	0	19	0	0
4	A	78	0	0	1	0
4	B	69	0	0	4	0
4	C	39	0	0	1	0
4	D	30	0	0	0	0
All	All	12462	0	12175	212	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 9.

All (212) 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:38:ARG:HH11	1:A:38:ARG:HG2	0.96	1.10
1:D:337:GLY:HA2	1:D:338:GLU:HB2	1.51	0.92
1:A:38:ARG:CG	1:A:38:ARG:HH11	1.82	0.92
1:B:299:THR:O	1:B:300:ARG:HB2	1.72	0.89
1:C:173:GLY:HA2	1:C:201:SER:OG	1.72	0.89
1:A:38:ARG:NH1	1:A:38:ARG:HG2	1.75	0.88
1:D:407:GLU:O	1:D:409:GLY:N	2.07	0.88
1:A:315:VAL:O	1:A:319:ASN:HB2	1.79	0.82
1:B:395:THR:HG21	2:B:3:NAD:H72N	1.46	0.81
1:B:298:ILE:HG12	1:B:300:ARG:HH12	1.47	0.79
1:D:337:GLY:CA	1:D:338:GLU:HB2	2.13	0.78
1:A:396:GLN:O	1:A:397:MET:HB3	1.86	0.76
1:A:249:ALA:O	1:A:250:GLU:HB2	1.91	0.71
1:A:343:ILE:HD12	1:A:343:ILE:N	2.05	0.71
1:B:82:SER:HA	1:B:112:ASN:ND2	2.06	0.70
1:B:82:SER:HA	1:B:112:ASN:HD21	1.55	0.70
1:C:311:ARG:NE	4:C:476:HOH:O	2.25	0.70
1:B:298:ILE:CG1	1:B:300:ARG:HH12	2.05	0.69
1:C:129:ALA:HB1	1:C:134:GLU:HB3	1.75	0.68
1:B:308:ASP:OD1	1:B:311:ARG:HD2	1.94	0.67
1:C:316:LEU:HD13	1:C:363:THR:HG22	1.77	0.66
1:D:255:THR:O	1:D:259:VAL:HG22	1.95	0.66
1:C:49:LEU:HD13	1:C:71:VAL:CG2	2.26	0.66
1:D:246:GLU:O	1:D:247:SER:C	2.32	0.66
1:B:322:ALA:HB3	1:B:323:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ALA:O	1:D:326:LEU:HG	1.97	0.65
1:A:426:GLU:OE1	1:A:426:GLU:HA	1.98	0.64
1:D:278:SER:HB3	1:D:282:ARG:HH21	1.63	0.64
1:A:401:ILE:O	1:A:406:ARG:NH1	2.31	0.63
1:C:41:GLU:HB2	1:C:42:PRO:HD2	1.80	0.63
1:A:268:VAL:HG22	2:A:1:NAD:N1A	2.13	0.63
1:A:223:ARG:HD2	4:A:500:HOH:O	1.98	0.62
1:A:295:ASN:HA	1:A:345:LEU:HD13	1.80	0.62
1:B:323:PRO:O	1:B:327:THR:HG22	1.99	0.62
1:D:259:VAL:HG23	1:D:261:GLY:H	1.64	0.61
1:B:219:THR:O	1:B:295:ASN:HB3	2.00	0.61
1:A:396:GLN:O	1:A:396:GLN:HG3	2.00	0.61
1:B:323:PRO:O	1:B:327:THR:CG2	2.50	0.60
1:A:25:GLN:HB3	1:B:22:LEU:HD11	1.83	0.60
1:B:344:GLY:HA3	4:B:520:HOH:O	2.01	0.58
1:A:414:SER:HB2	1:A:449:GLN:HB3	1.85	0.57
1:B:60:LEU:HD11	1:B:178:MET:HG3	1.85	0.57
1:A:322:ALA:HB3	1:A:323:PRO:HD3	1.86	0.57
1:C:132:THR:O	1:C:136:ILE:HG13	2.04	0.57
1:D:337:GLY:HA2	1:D:338:GLU:CB	2.32	0.57
1:B:298:ILE:CG1	1:B:300:ARG:NH1	2.67	0.57
1:C:103:HIS:HE1	1:D:307:MET:O	1.88	0.57
1:A:415:LEU:HD12	1:A:448:GLY:HA2	1.87	0.56
1:A:32:GLU:OE2	1:A:115:ARG:HG2	2.06	0.56
1:B:298:ILE:HG13	1:B:300:ARG:NH1	2.19	0.56
1:A:100:LYS:O	1:A:103:HIS:HB3	2.06	0.56
1:C:230:ALA:HB1	1:C:259:VAL:HG11	1.88	0.56
1:D:354:ASN:HB3	1:D:357:GLN:HG3	1.87	0.55
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.52	0.55
1:B:299:THR:O	1:B:300:ARG:CB	2.48	0.55
1:D:185:LYS:HB3	1:D:426:GLU:HG2	1.88	0.55
1:C:126:PRO:O	1:C:135:ARG:HG3	2.07	0.55
1:A:373:ALA:CB	1:B:135:ARG:HD3	2.37	0.54
1:C:413:ASN:HB3	1:C:450:ALA:HA	1.89	0.54
1:B:413:ASN:HB3	1:B:450:ALA:HA	1.89	0.54
1:D:172:THR:HB	1:D:201:SER:H	1.73	0.54
1:A:86:LEU:O	1:A:119:VAL:HA	2.07	0.54
1:C:49:LEU:CD1	1:C:71:VAL:HG22	2.37	0.54
1:C:189:VAL:HG22	1:C:446:VAL:HG22	1.90	0.54
1:C:49:LEU:HD13	1:C:71:VAL:HG22	1.89	0.54
1:B:314:ALA:O	1:B:318:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ALA:O	1:D:277:ILE:HG13	2.08	0.53
1:D:181:LEU:HD21	1:D:194:PHE:CZ	2.44	0.53
1:A:26:LEU:HD23	1:B:22:LEU:HD13	1.91	0.53
1:D:295:ASN:HA	1:D:345:LEU:HD13	1.90	0.52
1:B:107:THR:HB	1:B:108:PRO:HD3	1.91	0.52
1:D:48:LEU:HD11	1:D:87:VAL:HG23	1.91	0.52
1:B:226:GLY:HA2	1:B:229:ILE:HD12	1.90	0.52
1:C:135:ARG:HD3	1:D:373:ALA:CB	2.40	0.52
1:D:348:ILE:HD12	1:D:391:GLY:HA2	1.90	0.52
1:B:311:ARG:O	1:B:315:VAL:HG23	2.10	0.52
1:A:115:ARG:NH2	1:A:154:ARG:HD2	2.24	0.52
1:C:149:GLY:HA2	1:C:158:THR:HG23	1.91	0.51
1:A:373:ALA:HB2	1:B:135:ARG:HD3	1.92	0.51
1:D:317:ALA:HA	1:D:321:LEU:HB2	1.91	0.51
1:A:234:ALA:HB2	1:A:259:VAL:HB	1.92	0.51
1:D:188:TYR:HD2	1:D:446:VAL:HG12	1.76	0.51
1:A:295:ASN:HB2	1:A:345:LEU:HD13	1.91	0.51
1:B:56:VAL:O	1:B:60:LEU:HB2	2.11	0.51
1:C:315:VAL:HG12	1:C:363:THR:HG21	1.91	0.51
1:C:47:SER:HA	1:C:69:ASP:HB3	1.91	0.51
2:B:3:NAD:N7N	2:B:3:NAD:O1N	2.43	0.50
1:B:273:ALA:O	1:B:277:ILE:HG13	2.11	0.50
1:C:346:SER:O	1:C:347:SER:O	2.29	0.50
1:A:26:LEU:O	1:A:28:VAL:N	2.45	0.50
1:D:115:ARG:HB3	1:D:115:ARG:NH1	2.26	0.50
1:D:269:THR:HG21	1:D:317:ALA:HB1	1.94	0.50
1:A:102:LEU:HD13	1:A:144:PHE:CG	2.46	0.50
1:B:181:LEU:HD21	1:B:194:PHE:CZ	2.47	0.50
1:C:304:LEU:HD23	1:D:110:LEU:HD11	1.92	0.50
1:D:190:ASP:HB3	1:D:449:GLN:N	2.27	0.50
1:D:231:GLU:OE2	1:D:258:LYS:HD3	2.11	0.50
1:A:268:VAL:HG22	2:A:1:NAD:C6A	2.41	0.50
1:B:274:VAL:HG21	1:B:329:GLY:HA3	1.94	0.50
1:A:244:ASP:HB2	1:A:252:LEU:HD13	1.94	0.50
1:A:30:GLN:NE2	1:A:31:PRO:HD2	2.27	0.50
1:D:298:ILE:HD11	1:D:314:ALA:O	2.11	0.50
1:D:246:GLU:O	1:D:247:SER:O	2.30	0.49
1:C:107:THR:HB	1:C:108:PRO:HD3	1.93	0.49
1:D:347:SER:HB3	2:D:4:NAD:H6N	1.94	0.49
1:D:180:PHE:O	1:D:183:SER:OG	2.27	0.49
1:A:342:VAL:O	1:A:385:ILE:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:NH1	1:D:184:ALA:HB2	2.28	0.49
1:D:126:PRO:C	1:D:128:ALA:H	2.16	0.48
1:A:451:MET:O	1:B:452:ILE:HA	2.14	0.48
1:B:55:ARG:CZ	1:B:165:PRO:HA	2.44	0.48
1:B:58:GLU:HB2	4:B:505:HOH:O	2.14	0.47
1:C:225:ILE:HG22	1:C:229:ILE:HD11	1.96	0.47
1:A:86:LEU:HB2	1:A:119:VAL:HG22	1.95	0.47
1:A:319:ASN:HB3	1:A:363:THR:CB	2.45	0.47
1:A:319:ASN:HB3	1:A:363:THR:HB	1.96	0.47
1:D:402:PRO:O	1:D:405:THR:HB	2.14	0.47
1:A:145:THR:HG21	1:A:160:LEU:HB2	1.97	0.47
1:D:115:ARG:CZ	1:D:115:ARG:HB3	2.46	0.46
1:D:244:ASP:HB2	1:D:252:LEU:HD13	1.97	0.46
1:A:181:LEU:HD21	1:A:194:PHE:CZ	2.50	0.46
1:D:311:ARG:O	1:D:315:VAL:HG23	2.15	0.46
1:A:413:ASN:HB3	1:A:450:ALA:HA	1.97	0.46
1:D:259:VAL:HG23	1:D:261:GLY:N	2.31	0.46
1:C:299:THR:HG22	1:C:360:TYR:CD1	2.50	0.46
1:C:401:ILE:H	1:C:401:ILE:HD13	1.81	0.46
1:A:295:ASN:CB	1:A:345:LEU:HD13	2.45	0.46
1:A:342:VAL:HG12	1:A:385:ILE:HG13	1.96	0.46
1:C:408:VAL:O	1:C:412:LEU:HB2	2.15	0.46
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.81	0.46
1:C:119:VAL:O	1:C:158:THR:HA	2.16	0.45
1:B:210:PRO:HD2	1:B:236:ASP:HB3	1.97	0.45
1:A:123:GLY:O	1:A:162:TYR:HA	2.16	0.45
1:C:35:ARG:NH2	1:C:42:PRO:O	2.50	0.45
1:C:422:VAL:O	1:C:426:GLU:HG2	2.16	0.45
1:B:291:ILE:HA	1:B:341:ARG:O	2.16	0.45
1:B:258:LYS:HE2	4:B:500:HOH:O	2.16	0.45
1:B:298:ILE:HD12	1:B:298:ILE:HA	1.89	0.45
1:D:210:PRO:HD2	1:D:236:ASP:HB3	1.99	0.45
1:A:229:ILE:HD13	1:A:293:VAL:HG11	1.99	0.45
1:C:54:GLY:HA3	1:C:91:THR:OG1	2.17	0.44
1:C:410:ARG:HG3	1:C:418:GLY:H	1.82	0.44
1:A:415:LEU:HD12	1:A:448:GLY:CA	2.46	0.44
1:C:373:ALA:HB2	1:D:135:ARG:HG2	1.99	0.44
1:A:175:GLU:HG2	1:A:179:ARG:HD2	1.99	0.44
1:A:407:GLU:OE2	1:A:411:ARG:HD3	2.16	0.44
1:B:253:ALA:O	1:B:257:SER:HB2	2.17	0.44
1:C:405:THR:O	1:C:405:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLY:HA2	1:C:244:ASP:OD1	2.18	0.44
1:C:361:ALA:CB	1:D:147:SER:OG	2.66	0.44
1:C:95:GLU:N	1:C:95:GLU:OE1	2.50	0.43
1:C:106:PHE:O	1:C:107:THR:C	2.56	0.43
1:C:120:VAL:HG22	1:C:159:ALA:HB3	1.99	0.43
1:C:346:SER:HA	1:C:364:LYS:HE3	2.00	0.43
1:A:244:ASP:OD2	2:A:1:NAD:H1B	2.17	0.43
1:A:288:LYS:NZ	1:A:334:GLY:O	2.51	0.43
1:A:390:PRO:HB2	2:A:1:NAD:C5N	2.49	0.43
1:B:37:TYR:CE2	1:B:235:ARG:HD2	2.54	0.43
1:D:388:VAL:HG21	1:D:428:ILE:HG13	1.98	0.43
1:A:386:ASN:OD1	1:A:442:ASN:HB2	2.19	0.43
1:B:208:GLU:C	1:B:210:PRO:HD3	2.38	0.43
1:D:318:VAL:O	1:D:323:PRO:HD3	2.18	0.43
1:C:55:ARG:O	1:C:59:PRO:HG2	2.17	0.43
1:B:57:VAL:O	1:B:61:ARG:HG3	2.17	0.43
1:D:312:TRP:CE3	1:D:359:ASN:HB3	2.54	0.43
1:A:314:ALA:O	1:A:318:VAL:HG23	2.18	0.43
1:C:354:ASN:O	1:D:147:SER:HB3	2.19	0.43
1:D:320:LEU:C	1:D:323:PRO:HD2	2.40	0.43
1:A:317:ALA:HA	1:A:321:LEU:HB2	2.02	0.42
1:B:452:ILE:HD13	1:B:452:ILE:HG21	1.78	0.42
1:C:307:MET:O	1:D:103:HIS:HE1	2.02	0.42
1:A:273:ALA:O	1:A:277:ILE:HG13	2.20	0.42
1:B:223:ARG:HD3	2:B:3:NAD:O2A	2.19	0.42
1:D:234:ALA:HA	1:D:238:ALA:O	2.19	0.42
1:D:57:VAL:HG13	1:D:58:GLU:HG2	2.00	0.42
1:D:59:PRO:HG3	1:D:169:PRO:O	2.19	0.42
1:B:97:ALA:O	1:B:100:LYS:HG2	2.19	0.42
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.91	0.42
1:B:357:GLN:HB3	1:B:360:TYR:HB3	2.02	0.42
1:C:268:VAL:HG22	2:C:2:NAD:N1A	2.34	0.41
1:D:207:TRP:O	1:D:210:PRO:HG3	2.20	0.41
1:A:295:ASN:CA	1:A:345:LEU:HD13	2.48	0.41
1:C:357:GLN:HB3	1:C:360:TYR:HB3	2.02	0.41
1:C:78:ARG:O	1:C:79:TRP:CB	2.67	0.41
1:D:90:ALA:HB1	1:D:93:ILE:HD12	2.01	0.41
1:B:142:GLU:OE2	1:B:146:ARG:NE	2.40	0.41
1:A:26:LEU:CD2	1:B:22:LEU:HD13	2.50	0.41
1:C:126:PRO:HD3	1:C:162:TYR:CE1	2.55	0.41
1:A:26:LEU:HD23	1:B:22:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ALA:HA	1:C:321:LEU:HB2	2.02	0.41
1:A:37:TYR:CD1	1:A:185:LYS:HE2	2.54	0.41
1:C:37:TYR:CD1	1:C:185:LYS:HE3	2.56	0.41
1:B:106:PHE:CE1	1:B:119:VAL:HG13	2.56	0.41
1:B:394:GLU:H	1:B:394:GLU:HG2	1.66	0.41
1:C:343:ILE:HA	1:C:386:ASN:O	2.20	0.41
1:C:95:GLU:HB2	1:C:96:PRO:HD2	2.02	0.41
1:D:268:VAL:HB	1:D:326:LEU:HD11	2.02	0.41
1:B:229:ILE:HA	1:B:425:ALA:HB1	2.03	0.41
1:D:324:LEU:HD13	1:D:370:ILE:HG12	2.01	0.41
1:A:249:ALA:HB2	1:A:265:TRP:CD1	2.56	0.41
1:B:217:ILE:HD11	1:B:281:LEU:HD11	2.03	0.41
1:A:348:ILE:HD12	1:A:391:GLY:HA2	2.03	0.41
1:A:58:GLU:HB3	1:A:59:PRO:HD3	2.02	0.41
1:B:317:ALA:HA	1:B:321:LEU:HB2	2.02	0.41
1:D:240:VAL:O	1:D:262:THR:N	2.52	0.41
1:A:71:VAL:HA	1:A:72:GLY:HA2	1.75	0.40
1:C:388:VAL:HG21	1:C:428:ILE:CG1	2.52	0.40
1:B:81:ASP:CB	4:B:514:HOH:O	2.68	0.40
1:D:375:ALA:N	1:D:376:PRO:HD2	2.37	0.40
1:A:35:ARG:CZ	1:A:45:THR:HG23	2.51	0.40
1:B:126:PRO:O	1:B:135:ARG:HG3	2.21	0.40
1:C:127:GLU:OE1	1:C:127:GLU:N	2.45	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	423/446 (95%)	398 (94%)	22 (5%)	3 (1%)	22 43
1	B	417/446 (94%)	393 (94%)	21 (5%)	3 (1%)	22 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	412/446 (92%)	384 (93%)	22 (5%)	6 (2%)	10	21
1	D	399/446 (90%)	364 (91%)	30 (8%)	5 (1%)	12	24
All	All	1651/1784 (92%)	1539 (93%)	95 (6%)	17 (1%)	15	32

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLU
1	B	300	ARG
1	C	347	SER
1	A	397	MET
1	C	39	ALA
1	C	40	GLY
1	C	45	THR
1	D	337	GLY
1	B	346	SER
1	B	347	SER
1	D	116	CYS
1	C	79	TRP
1	D	97	ALA
1	D	100	LYS
1	D	305	ALA
1	A	27	GLY
1	C	72	GLY

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	306/323 (95%)	287 (94%)	19 (6%)	18	37
1	B	303/323 (94%)	289 (95%)	14 (5%)	27	51
1	C	292/323 (90%)	279 (96%)	13 (4%)	27	52
1	D	287/323 (89%)	267 (93%)	20 (7%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1188/1292 (92%)	1122 (94%)	66 (6%)	21	42

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	25	GLN
1	A	26	LEU
1	A	28	VAL
1	A	38	ARG
1	A	41	GLU
1	A	45	THR
1	A	71	VAL
1	A	95	GLU
1	A	127	GLU
1	A	244	ASP
1	A	247	SER
1	A	251	ASN
1	A	302	LYS
1	A	343	ILE
1	A	345	LEU
1	A	397	MET
1	A	411	ARG
1	A	430	TYR
1	B	20	SER
1	B	30	GLN
1	B	58	GLU
1	B	244	ASP
1	B	262	THR
1	B	266	LEU
1	B	271	ASP
1	B	276	LYS
1	B	288	LYS
1	B	300	ARG
1	B	327	THR
1	B	348	ILE
1	B	403	LEU
1	B	430	TYR
1	C	69	ASP
1	C	71	VAL
1	C	74	ASN
1	C	195	SER

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Mol	Chain	Res	Type
1	C	201	SER
1	C	223	ARG
1	C	258	LYS
1	C	321	LEU
1	C	401	ILE
1	C	405	THR
1	C	407	GLU
1	C	408	VAL
1	C	430	TYR
1	D	33	THR
1	D	45	THR
1	D	172	THR
1	D	208	GLU
1	D	212	ASP
1	D	246	GLU
1	D	247	SER
1	D	258	LYS
1	D	262	THR
1	D	265	TRP
1	D	275	ASP
1	D	282	ARG
1	D	309	ASP
1	D	316	LEU
1	D	394	GLU
1	D	395	THR
1	D	401	ILE
1	D	426	GLU
1	D	430	TYR
1	D	433	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	103	HIS
1	A	192	GLN
1	A	251	ASN
1	A	294	ASN
1	B	30	GLN
1	B	112	ASN
1	B	239	HIS
1	B	284	HIS

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Mol	Chain	Res	Type
1	C	103	HIS
1	C	192	GLN
1	C	251	ASN
1	C	284	HIS
1	C	420	GLN
1	D	294	ASN
1	D	357	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	NAD	B	3	-	42,48,48	1.87	4 (9%)	50,73,73	1.39	3 (6%)
2	NAD	C	2	-	42,48,48	1.90	4 (9%)	50,73,73	1.35	3 (6%)
2	NAD	A	1	-	42,48,48	1.87	6 (14%)	50,73,73	1.52	5 (10%)
2	NAD	D	4	-	42,48,48	1.85	4 (9%)	50,73,73	1.37	5 (10%)
3	ZPG	A	455	-	9,12,28	0.82	0	10,14,34	1.37	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	3	-	-	10/26/62/62	0/5/5/5
2	NAD	C	2	-	-	7/26/62/62	0/5/5/5
2	NAD	A	1	-	-	2/26/62/62	0/5/5/5
2	NAD	D	4	-	-	5/26/62/62	0/5/5/5
3	ZPG	A	455	-	-	2/12/12/31	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	NAD	O7N-C7N	9.85	1.43	1.24
2	C	2	NAD	O7N-C7N	9.65	1.42	1.24
2	D	4	NAD	O7N-C7N	9.45	1.42	1.24
2	A	1	NAD	O7N-C7N	9.20	1.41	1.24
2	D	4	NAD	C2A-N3A	4.16	1.38	1.32
2	C	2	NAD	C2A-N3A	4.03	1.38	1.32
2	B	3	NAD	C2A-N3A	4.03	1.38	1.32
2	A	1	NAD	C2N-N1N	3.76	1.39	1.35
2	A	1	NAD	C2A-N3A	3.24	1.37	1.32
2	C	2	NAD	C2N-N1N	3.10	1.38	1.35
2	B	3	NAD	C2N-N1N	2.57	1.38	1.35
2	D	4	NAD	C2A-N1A	2.57	1.38	1.33
2	B	3	NAD	C2A-N1A	2.54	1.38	1.33
2	D	4	NAD	C2N-N1N	2.47	1.38	1.35
2	A	1	NAD	C2A-N1A	2.39	1.38	1.33
2	C	2	NAD	C2A-N1A	2.39	1.38	1.33
2	A	1	NAD	O4D-C4D	-2.27	1.39	1.45
2	A	1	NAD	C2N-C3N	2.03	1.42	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAD	N3A-C2A-N1A	-6.97	117.78	128.68
2	B	3	NAD	N3A-C2A-N1A	-6.14	119.08	128.68
2	C	2	NAD	N3A-C2A-N1A	-6.00	119.30	128.68
2	D	4	NAD	N3A-C2A-N1A	-5.10	120.70	128.68
2	D	4	NAD	C6N-N1N-C2N	-4.09	118.24	121.97
2	B	3	NAD	C6N-N1N-C2N	-3.79	118.52	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAD	C1B-N9A-C4A	-3.03	121.32	126.64
2	A	1	NAD	PN-O3-PA	-2.97	122.64	132.83
2	A	1	NAD	C1B-N9A-C4A	-2.81	121.71	126.64
2	D	4	NAD	C2N-N1N-C1D	2.44	124.57	119.14
2	D	4	NAD	C3D-C2D-C1D	2.39	104.58	100.98
3	A	455	ZPG	O20-C20-C18	2.35	114.89	108.64
2	A	1	NAD	C2A-N1A-C6A	2.33	122.74	118.75
2	D	4	NAD	C3B-C2B-C1B	2.31	104.45	100.98
2	C	2	NAD	C6N-N1N-C2N	-2.30	119.88	121.97
2	B	3	NAD	C1B-N9A-C4A	-2.19	122.80	126.64
3	A	455	ZPG	C21-O20-C20	2.18	118.27	115.02
2	A	1	NAD	O7N-C7N-N7N	-2.15	119.52	122.58

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	NAD	C5B-O5B-PA-O1A
2	B	3	NAD	C5B-O5B-PA-O2A
2	B	3	NAD	C5D-O5D-PN-O3
2	C	2	NAD	C5D-O5D-PN-O3
2	C	2	NAD	C5D-O5D-PN-O2N
2	C	2	NAD	O4D-C4D-C5D-O5D
2	A	1	NAD	O4D-C1D-N1N-C2N
2	D	4	NAD	C4B-C5B-O5B-PA
2	D	4	NAD	O4B-C4B-C5B-O5B
2	D	4	NAD	C5D-O5D-PN-O3
2	C	2	NAD	C3D-C4D-C5D-O5D
2	D	4	NAD	C3B-C4B-C5B-O5B
3	A	455	ZPG	C27-C24-O23-C22
2	B	3	NAD	O4D-C4D-C5D-O5D
2	B	3	NAD	PN-O3-PA-O5B
2	A	1	NAD	PN-O3-PA-O2A
2	B	3	NAD	C5D-O5D-PN-O1N
2	C	2	NAD	C5D-O5D-PN-O1N
2	D	4	NAD	C5D-O5D-PN-O1N
2	B	3	NAD	PN-O3-PA-O1A
3	A	455	ZPG	C25-C20-O20-C21
2	B	3	NAD	C3D-C4D-C5D-O5D
2	B	3	NAD	C5B-O5B-PA-O3
2	C	2	NAD	O4B-C4B-C5B-O5B
2	C	2	NAD	PA-O3-PN-O1N

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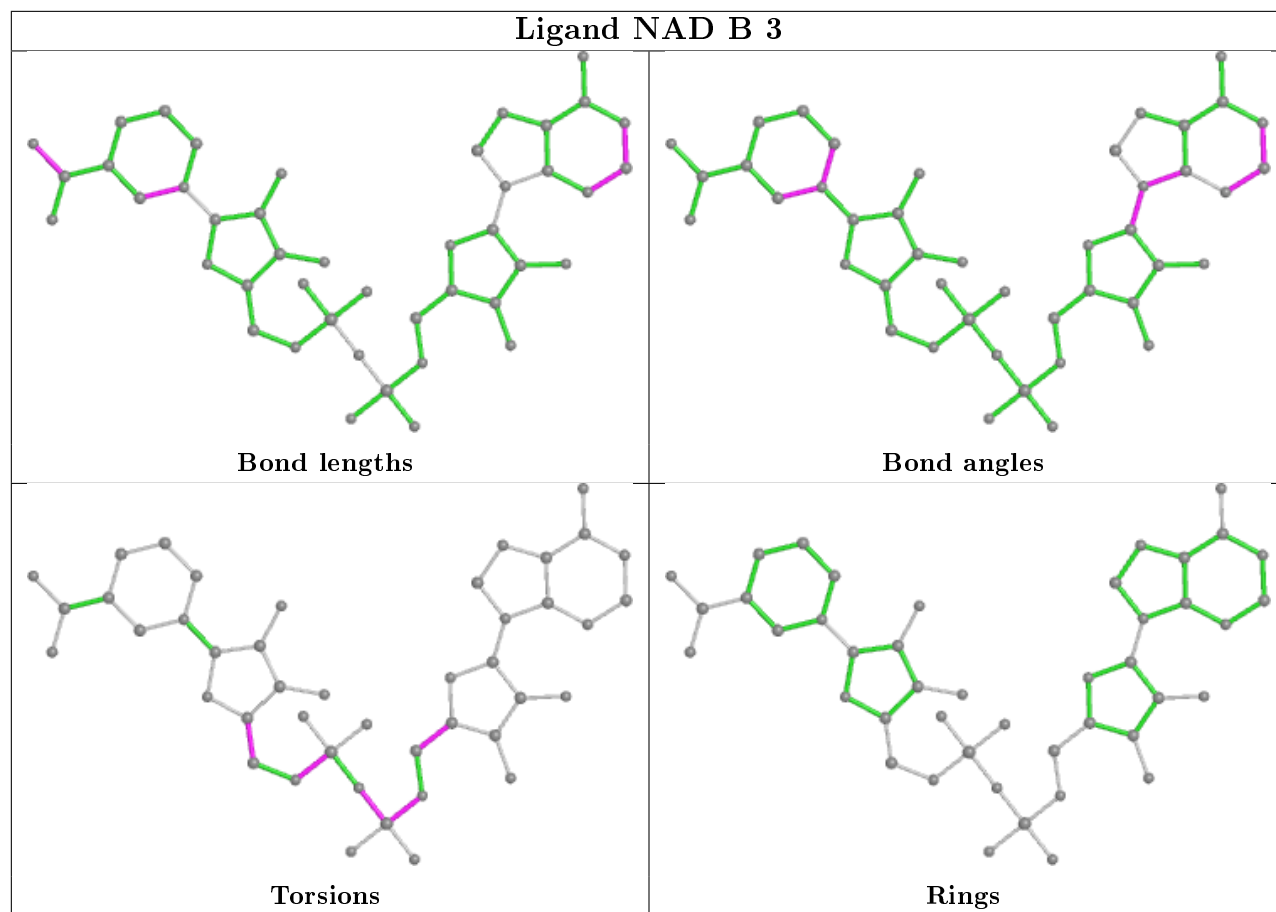
Mol	Chain	Res	Type	Atoms
2	B	3	NAD	O4B-C4B-C5B-O5B

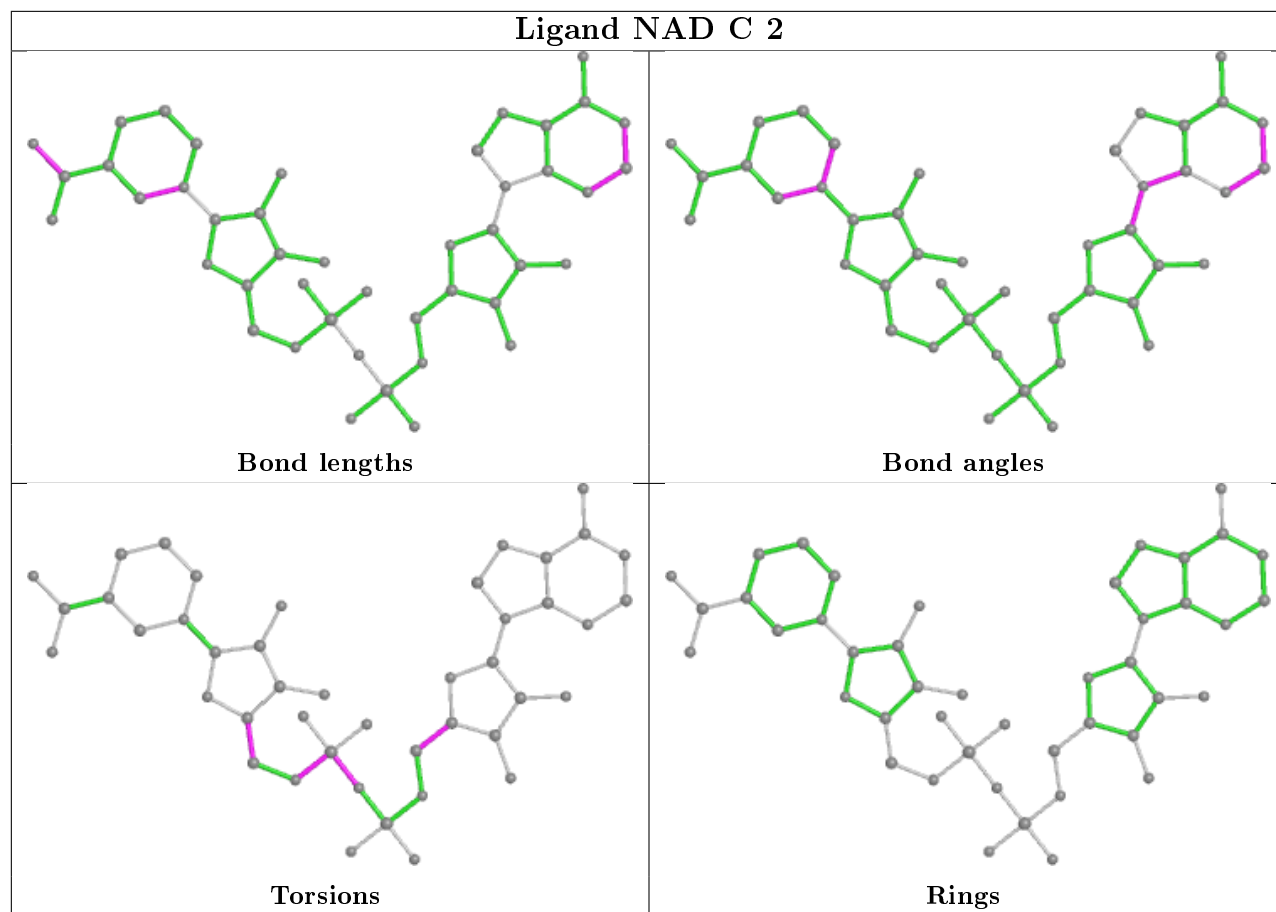
There are no ring outliers.

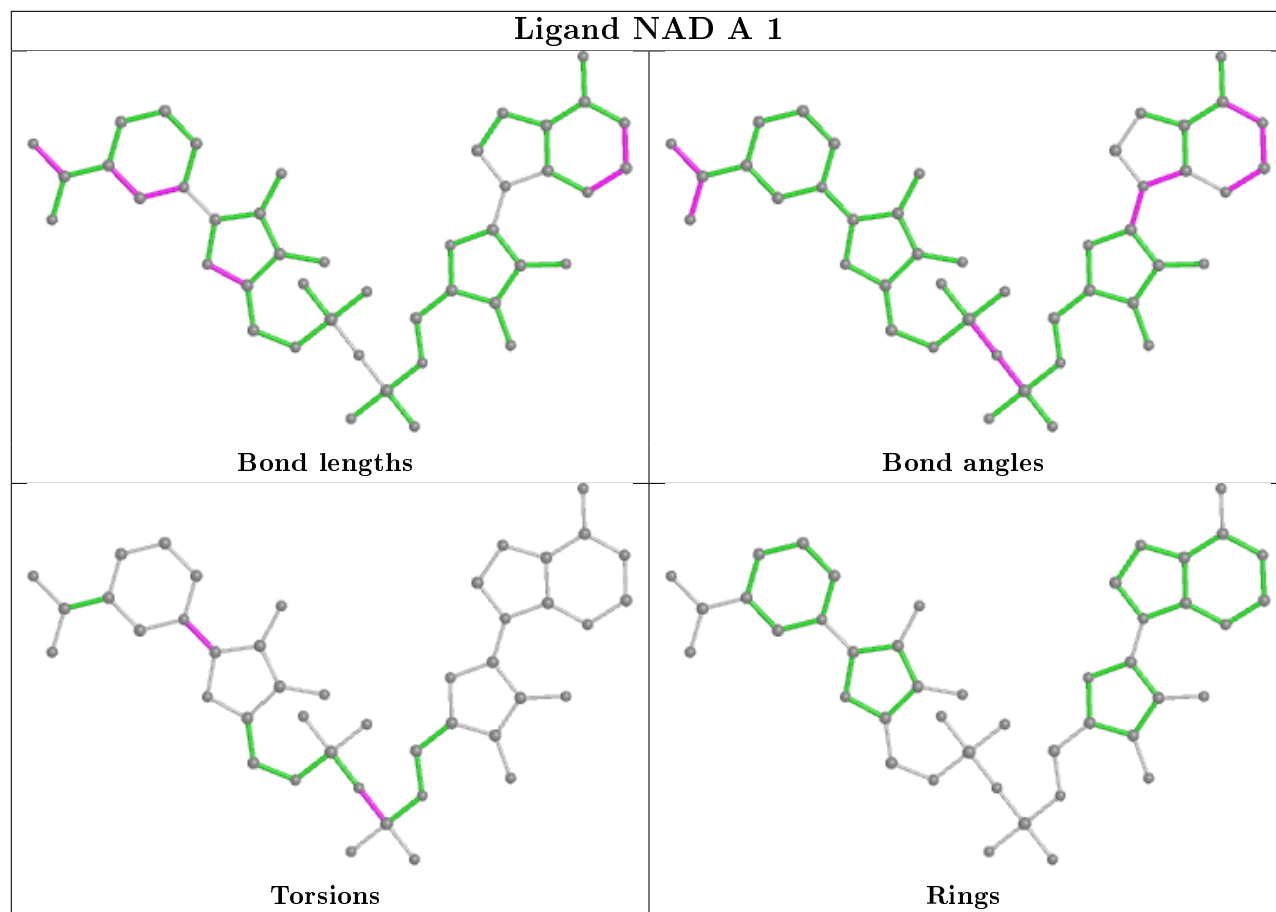
4 monomers are involved in 9 short contacts:

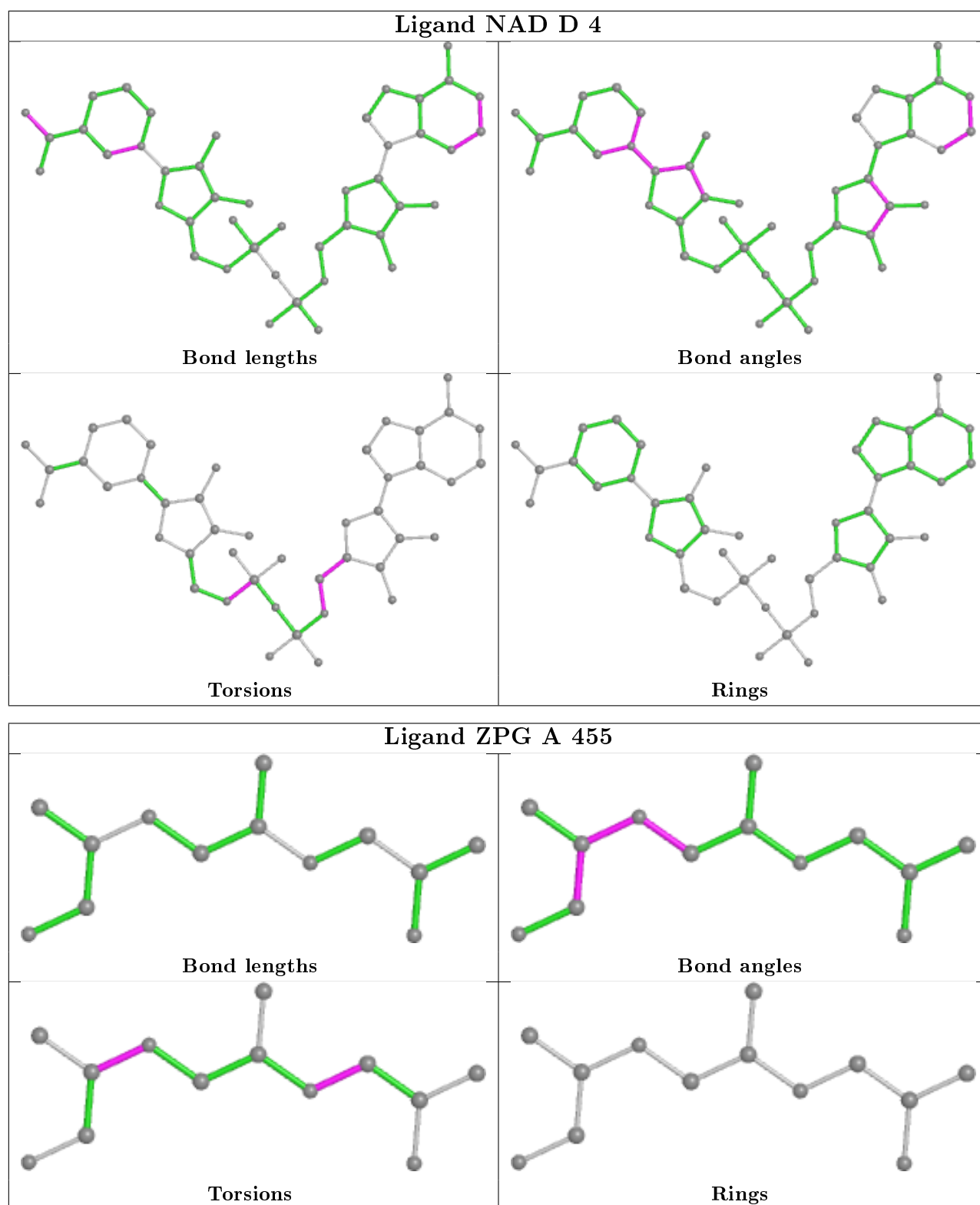
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	NAD	3	0
2	C	2	NAD	1	0
2	A	1	NAD	4	0
2	D	4	NAD	1	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/446 (95%)	-0.16	4 (0%) 84 82	17, 33, 54, 67	0
1	B	425/446 (95%)	-0.01	11 (2%) 56 50	14, 36, 71, 83	0
1	C	418/446 (93%)	-0.01	15 (3%) 42 35	19, 40, 66, 78	0
1	D	409/446 (91%)	0.41	32 (7%) 13 9	27, 52, 88, 103	0
All	All	1679/1784 (94%)	0.06	62 (3%) 41 34	14, 40, 75, 103	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	400	ALA	6.1
1	D	72	GLY	5.2
1	D	239	HIS	4.3
1	D	81	ASP	4.2
1	D	272	ASP	4.2
1	D	217	ILE	4.0
1	D	243	ILE	3.8
1	D	71	VAL	3.7
1	C	405	THR	3.7
1	D	241	VAL	3.6
1	D	30	GLN	3.3
1	D	404	ALA	3.3
1	B	30	GLN	3.3
1	D	29	PRO	3.2
1	C	130	ALA	3.2
1	C	40	GLY	3.1
1	B	246	GLU	3.0
1	D	379	ALA	3.0
1	C	29	PRO	2.9
1	D	223	ARG	2.9
1	C	404	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	265	TRP	2.8
1	D	292	LEU	2.8
1	D	380	ALA	2.7
1	B	81	ASP	2.6
1	B	223	ARG	2.6
1	C	39	ALA	2.6
1	A	243	ILE	2.6
1	A	40	GLY	2.6
1	D	310	ALA	2.5
1	D	262	THR	2.5
1	B	218	VAL	2.5
1	C	282	ARG	2.5
1	C	401	ILE	2.5
1	A	72	GLY	2.5
1	D	218	VAL	2.4
1	C	286	GLY	2.4
1	B	283	ASP	2.4
1	D	42	PRO	2.4
1	D	245	VAL	2.4
1	B	72	GLY	2.4
1	D	270	ALA	2.4
1	D	407	GLU	2.4
1	D	333	ASN	2.3
1	B	217	ILE	2.2
1	C	408	VAL	2.2
1	B	284	HIS	2.2
1	D	205	ALA	2.2
1	D	271	ASP	2.2
1	C	380	ALA	2.2
1	D	33	THR	2.2
1	D	405	THR	2.1
1	D	216	ALA	2.1
1	A	41	GLU	2.1
1	D	265	TRP	2.1
1	C	30	GLN	2.1
1	B	243	ILE	2.1
1	D	251	ASN	2.1
1	D	403	LEU	2.1
1	D	41	GLU	2.1
1	C	42	PRO	2.0
1	C	41	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 carbohydrates in this entry.

6.4 Ligands [i](#)

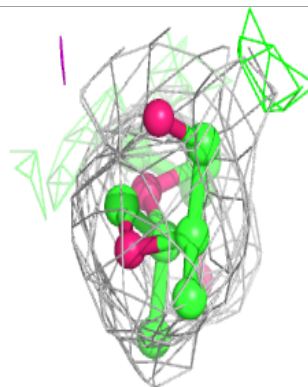
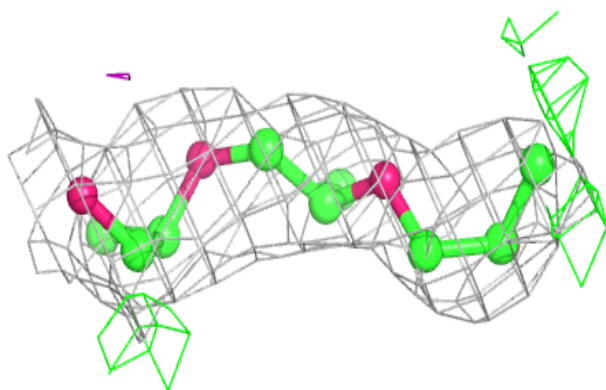
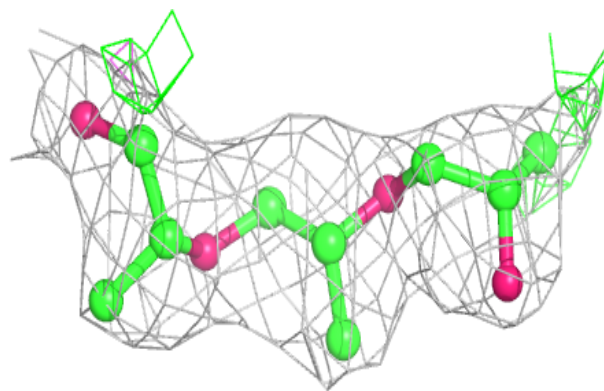
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZPG	A	455	13/29	0.85	0.17	60,63,66,67	0
2	NAD	D	4	44/44	0.93	0.15	54,66,71,74	0
2	NAD	B	3	44/44	0.93	0.17	55,62,70,71	0
2	NAD	C	2	44/44	0.95	0.13	39,46,53,55	0
2	NAD	A	1	44/44	0.95	0.13	30,36,46,50	0

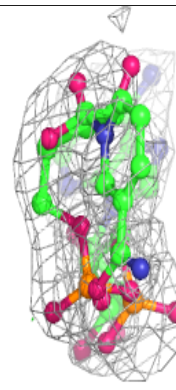
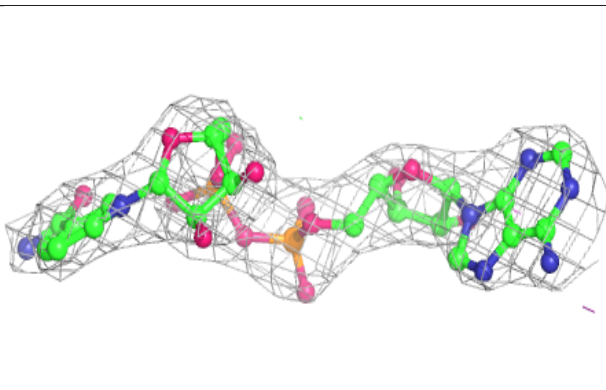
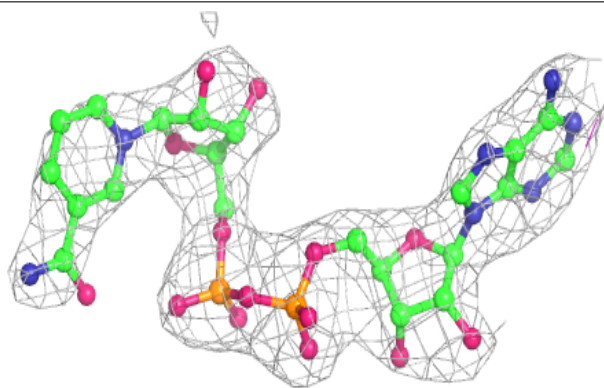
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZPG A 455:

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

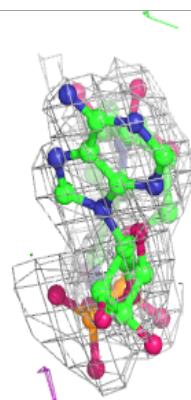
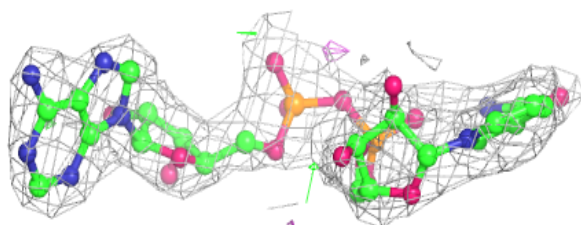
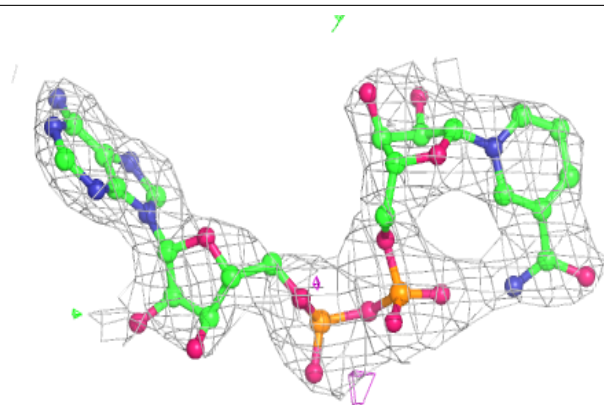
**Electron density around NAD D 4:**

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

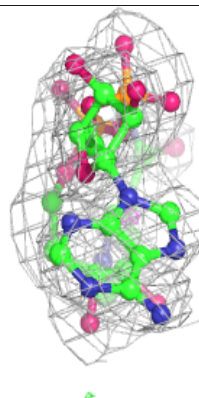
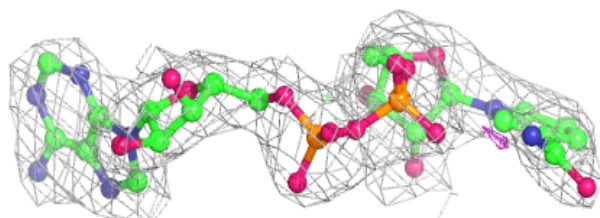
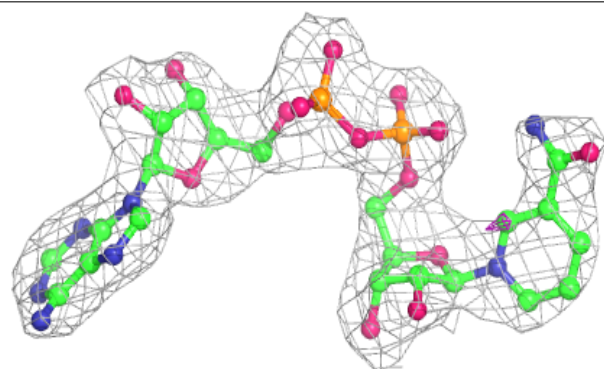


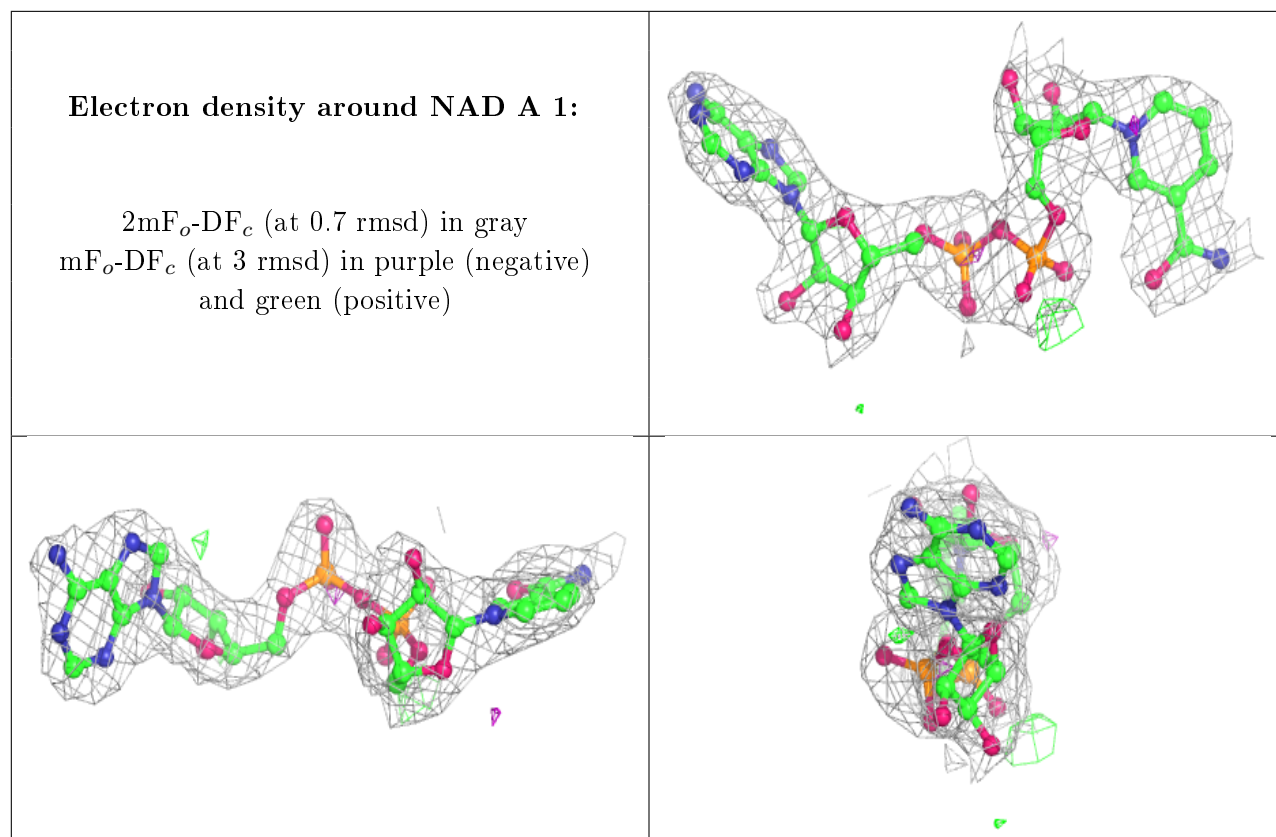
Electron density around NAD B 3:

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

**Electron density around NAD C 2:**

$2mF_o-DF_c$ (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.