



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:00 PM UTC

PDB ID : 9C36 / pdb_00009c36
Title : Proline utilization A complexed with the substrate L-glutamate gamma-semialdehyde in the aldehyde dehydrogenase active site
Authors : Tanner, J.J.; Buckley, D.P.
Deposited on : 2024-05-31
Resolution : 1.47 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

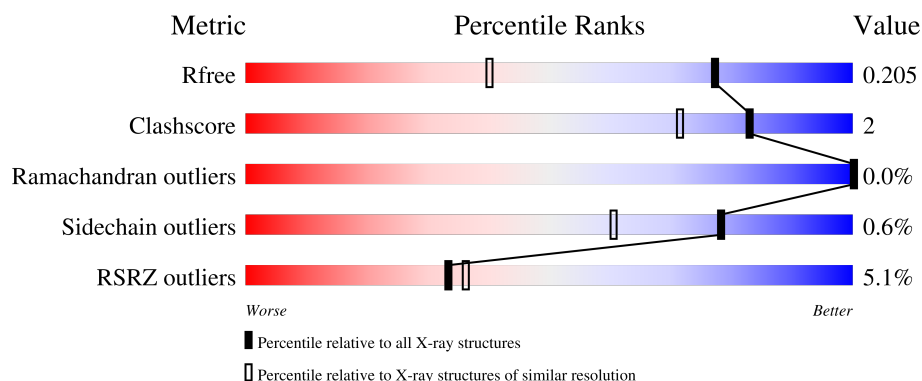
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	1235	4% 93% 5%
1	B	1235	6% 92% 5%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 37779 atoms, of which 17914 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.

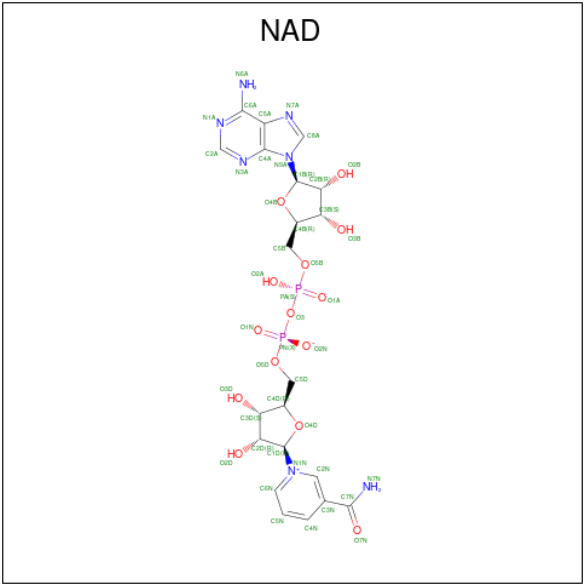
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1210	Total	C	H	N	O	S	0	7	0
			17790	5616	8877	1591	1674	32			
1	B	1209	Total	C	H	N	O	S	0	9	0
			17734	5603	8839	1586	1674	32			

There are 6 discrepancies between the modelled and reference sequences:

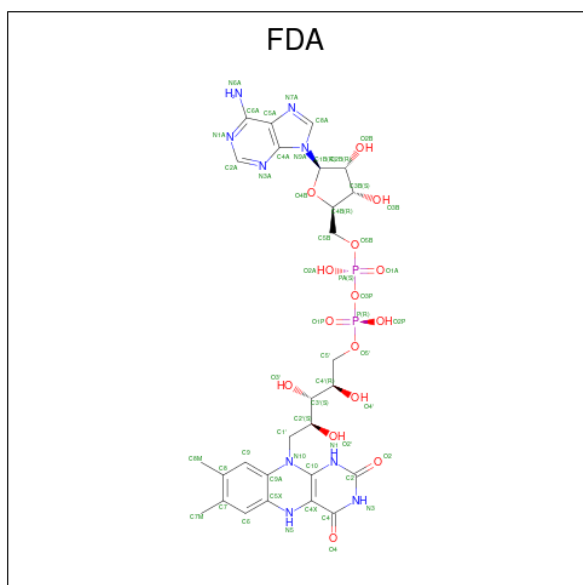
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
A	844	SER	CYS	engineered mutation	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3
B	844	SER	CYS	engineered mutation	UNP F7X6I3

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



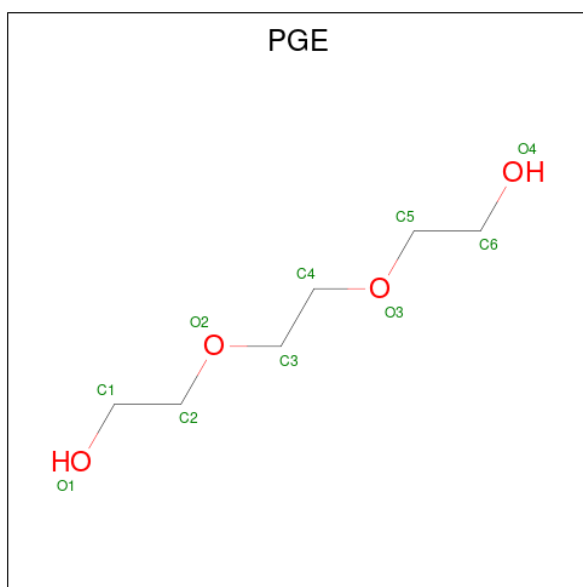
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	1
			140	42	52	14	28	4		

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



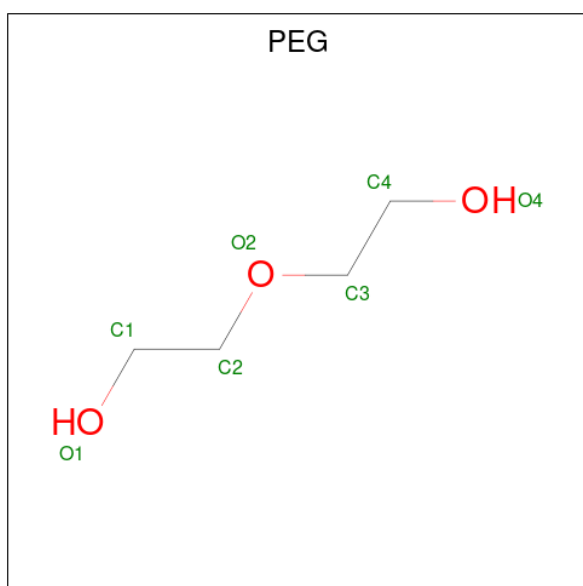
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
3	B	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		
4	B	1	Total	C	H	O	0	0
			24	6	14	4		

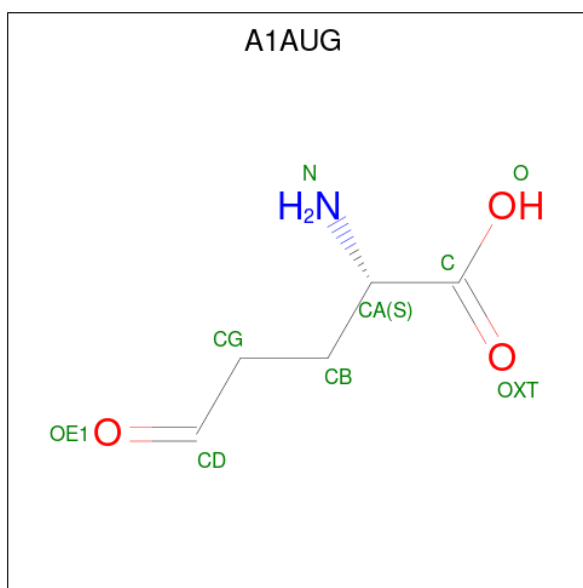
- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		

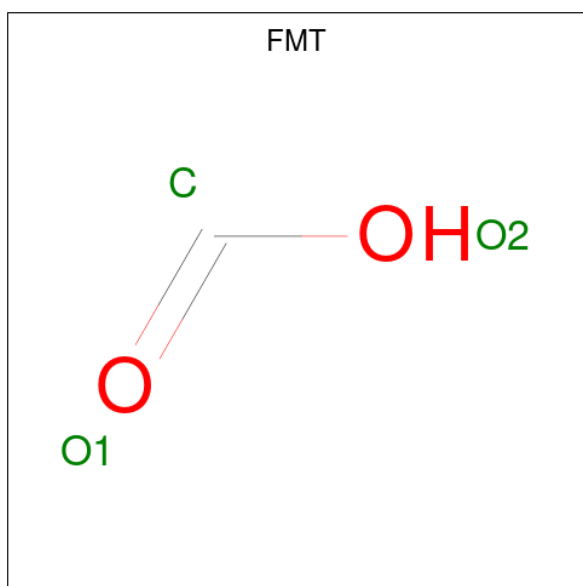
- Molecule 6 is 5-oxo-L-norvaline (CCD ID: A1AUG) (formula: $C_5H_9NO_3$) (labeled as "Ligand

of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			17	5	8	1	3		
6	B	1	Total	C	H	N	O	0	0
			17	5	8	1	3		

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			4	1	1	2		

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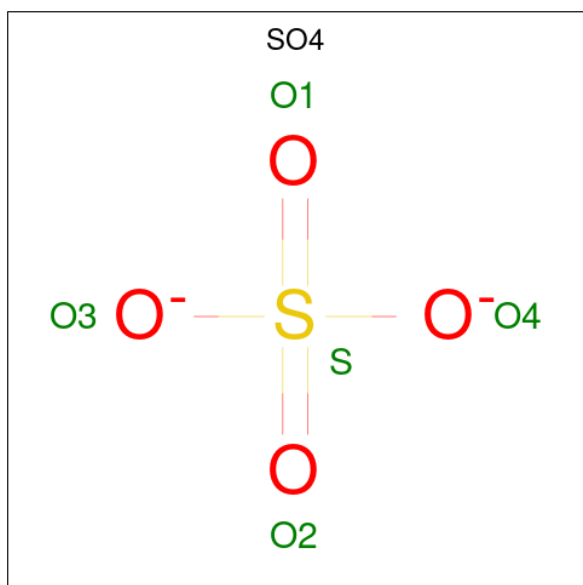
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			4	1	1	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Mg	0	0
			2	2		
8	B	1	Total	Mg	0	1
			2	2		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

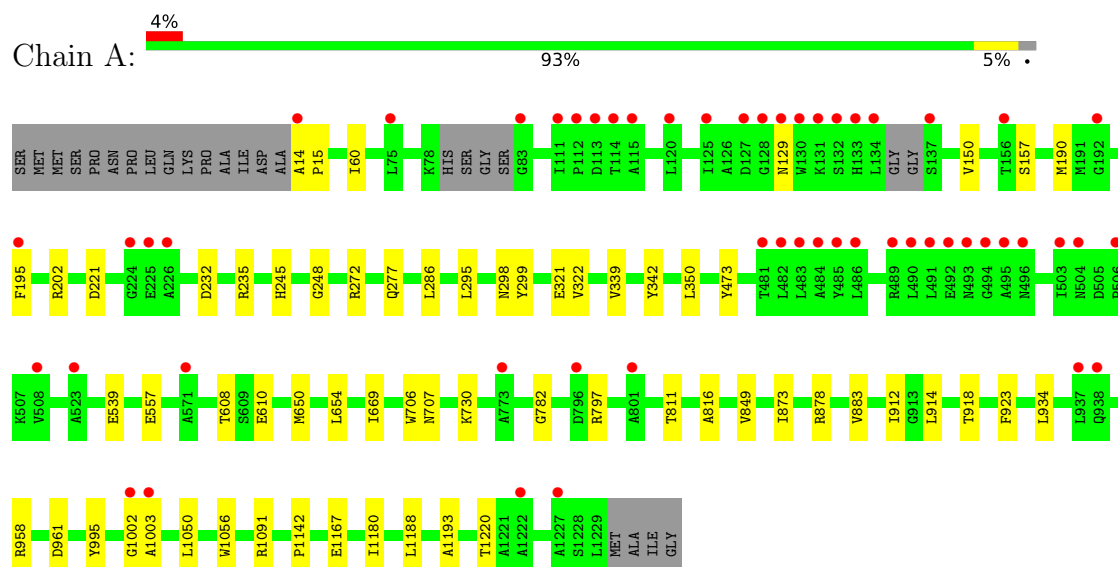
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	870	Total 870	O 870	0	0
10	B	864	Total 864	O 864	0	1

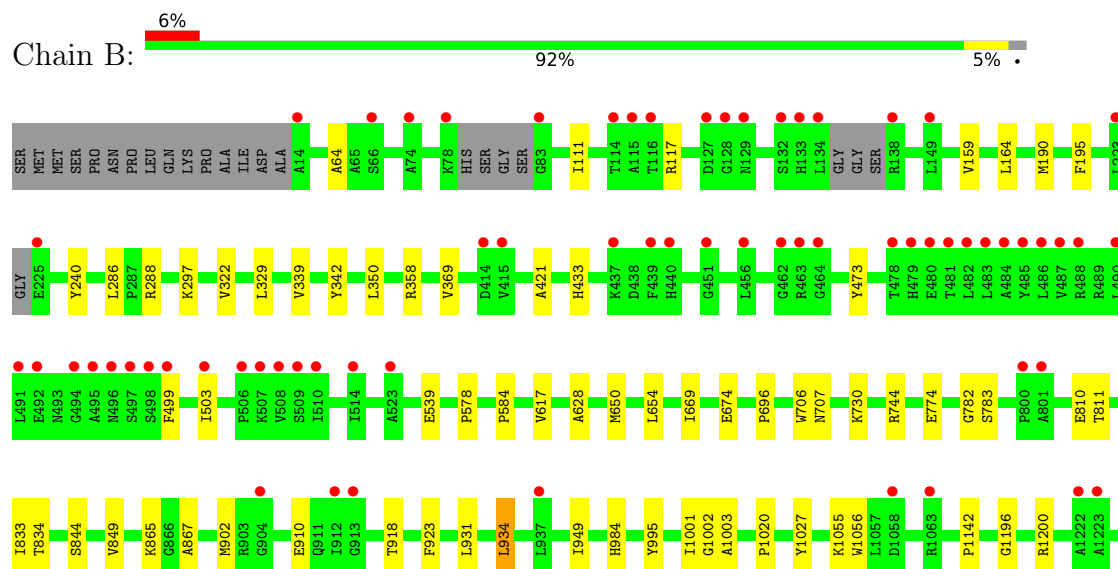
3 Residue-property plots [i](#)

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: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA



•	•	•	•
S1227	S1228	L1229	M1230
ALA	ILE	GLY	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.87Å 101.82Å 126.03Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	48.35 – 1.47 48.35 – 1.47	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.35-1.47) 97.6 (48.35-1.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.47Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.180 , 0.207 0.179 , 0.205	Depositor DCC
R_{free} test set	20070 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37779	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, MG, FMT, A1AUG, PGE, FDA, SO4, PEG

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	0.42	0/9083	0.56	0/12376
1	B	0.43	0/9069	0.58	0/12358
All	All	0.43	0/18152	0.57	0/24734

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	744	ARG	Sidechain

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	8913	8877	8867	38	0
1	B	8895	8839	8829	44	0
2	A	44	26	26	0	0
2	B	88	52	52	3	0
3	A	53	32	33	3	0
3	B	53	32	32	1	0
4	A	10	14	14	0	0
4	B	10	14	14	0	0
5	A	7	10	10	0	0
6	A	9	8	0	1	0
6	B	9	8	0	2	0
7	A	3	1	1	0	0
7	B	3	1	1	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	20	0	0	0	0
9	B	10	0	0	0	0
10	A	870	0	0	9	0
10	B	864	0	0	11	0
All	All	19865	17914	17879	85	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 2.

All (85) 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:539:GLU:OE1	10:A:2201:HOH:O	1.97	0.81
1:B:995:TYR:OH	1:B:1002[B]:GLY:O	2.01	0.79
1:A:995:TYR:OH	1:A:1002[A]:GLY:O	2.06	0.72
1:A:557:GLU:OE2	10:A:2203:HOH:O	2.09	0.70
1:A:232:ASP:OD2	10:A:2202:HOH:O	2.08	0.70
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.74	0.69
1:A:298:ASN:OD1	10:A:2204:HOH:O	2.10	0.68
1:B:783:SER:HB3	2:B:2205[B]:NAD:O4D	1.96	0.66
1:B:539:GLU:OE1	10:B:2301:HOH:O	2.14	0.65
1:A:150:VAL:HG11	1:A:190:MET:HE1	1.81	0.62
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.82	0.61
1:B:810:GLU:CD	10:B:2396:HOH:O	2.44	0.60
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.83	0.60
1:B:674:GLU:OE2	10:B:2302:HOH:O	2.17	0.58
1:B:810:GLU:HG3	10:B:2396:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:HB2	3:A:2102:FDA:HM72	1.86	0.57
1:A:608:THR:O	10:A:2205:HOH:O	2.18	0.55
1:B:865:LYS:NZ	1:B:910:GLU:OE2	2.28	0.55
1:B:1003[B]:ALA:O	10:B:2303:HOH:O	2.18	0.54
1:A:650:MET:O	1:A:654:LEU:HG	2.07	0.54
1:B:288:ARG:NE	10:B:2317:HOH:O	2.40	0.54
1:A:232:ASP:OD1	1:A:235:ARG:NH1	2.36	0.53
1:A:1003[A]:ALA:O	10:A:2206:HOH:O	2.18	0.53
1:B:849:VAL:HG21	1:B:934:LEU:HD21	1.90	0.53
1:B:833:ILE:HD11	1:B:867:ALA:HB3	1.91	0.52
1:A:654:LEU:HD21	1:A:669:ILE:HA	1.91	0.51
1:A:1091:ARG:HG3	1:A:1220:THR:HG21	1.91	0.51
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.91	0.50
1:B:810:GLU:CG	10:B:2396:HOH:O	2.57	0.50
1:B:240:TYR:OH	10:B:2304:HOH:O	2.19	0.50
1:A:782:GLY:O	1:A:811:THR:HA	2.12	0.50
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.47	0.49
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.47	0.49
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.47	0.49
1:B:358:ARG:NH1	10:B:2308:HOH:O	2.31	0.49
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.93	0.49
6:B:2203:A1AUG:OE1	2:B:2205[A]:NAD:C5N	2.61	0.49
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.94	0.48
1:B:782:GLY:O	1:B:811:THR:HA	2.13	0.48
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.95	0.48
1:B:844:SER:H	6:B:2203:A1AUG:CD	2.26	0.48
1:A:150:VAL:CG1	1:A:190:MET:HE1	2.43	0.48
1:B:1196:GLY:O	1:B:1200:ARG:HG3	2.14	0.48
1:B:111:ILE:O	1:B:117:ARG:NH2	2.41	0.47
1:B:650:MET:O	1:B:654:LEU:HG	2.14	0.47
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.39	0.46
1:B:834:THR:HG22	1:B:1001[A]:ILE:HD11	1.98	0.46
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.51	0.46
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.40	0.45
2:B:2205[B]:NAD:O2N	10:B:2305:HOH:O	2.21	0.45
1:B:159:VAL:CG1	1:B:164:LEU:HD12	2.48	0.44
1:B:654:LEU:HD21	1:B:669:ILE:HA	2.00	0.44
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.51	0.44
1:A:878:ARG:HD2	10:A:2400:HOH:O	2.17	0.44
1:A:1167:GLU:HA	1:A:1193:ALA:O	2.18	0.44
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:ARG:O	1:A:961:ASP:HB2	2.18	0.43
1:B:918:THR:HB	1:B:923:PHE:CD1	2.53	0.43
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.53	0.42
1:B:706:TRP:CD2	1:B:706:TRP:C	2.97	0.42
1:A:221:ASP:HB2	1:A:473:TYR:CZ	2.55	0.42
1:B:369:VAL:HG12	1:B:421:ALA:HB3	2.01	0.42
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.55	0.42
1:A:202:ARG:NH2	10:A:2235:HOH:O	2.53	0.42
1:B:617:VAL:HG12	1:B:774:GLU:HB2	2.02	0.42
3:A:2102:FDA:H9	3:A:2102:FDA:O4'	2.20	0.41
3:A:2102:FDA:O2'	3:A:2102:FDA:N1	2.53	0.41
1:B:984:HIS:C	1:B:984:HIS:CD2	2.98	0.41
1:A:14:ALA:HA	1:A:15:PRO:HD3	1.96	0.41
1:A:816:ALA:HA	1:A:849:VAL:O	2.21	0.41
1:B:1003[B]:ALA:HB1	10:B:2303:HOH:O	2.21	0.41
1:A:272:ARG:HB3	1:A:277:GLN:HG3	2.01	0.41
1:B:190:MET:HE2	1:B:195:PHE:CZ	2.55	0.41
1:B:499:PHE:CZ	1:B:503:ILE:HD11	2.56	0.41
1:B:578:PRO:O	1:B:584:PRO:HA	2.21	0.41
1:A:60:ILE:HD12	10:A:2894:HOH:O	2.20	0.41
1:A:1003[A]:ALA:CB	6:A:2105:A1AUG:N	2.83	0.41
1:B:902:MET:HE3	1:B:931:LEU:CD2	2.51	0.41
1:B:499:PHE:CE1	1:B:503:ILE:HG13	2.55	0.40
1:B:628:ALA:HB2	1:B:696:PRO:HG3	2.03	0.40
1:B:833:ILE:HD11	1:B:867:ALA:CB	2.51	0.40
1:A:912:ILE:HD11	1:A:914:LEU:HD23	2.02	0.40
1:A:918:THR:HB	1:A:923:PHE:CD1	2.57	0.40
1:B:473:TYR:HB2	3:B:2201:FDA:HM72	2.02	0.40
1:B:1020:PRO:HG2	1:B:1027:TYR:HA	2.03	0.40

There are no symmetry-related clashes.

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	1211/1235 (98%)	1185 (98%)	25 (2%)	1 (0%)	48	23
1	B	1210/1235 (98%)	1178 (97%)	32 (3%)	0	100	100
All	All	2421/2470 (98%)	2363 (98%)	57 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ASN

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	885/951 (93%)	878 (99%)	7 (1%)	73	52
1	B	882/951 (93%)	878 (100%)	4 (0%)	81	65
All	All	1767/1902 (93%)	1756 (99%)	11 (1%)	78	60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	321	GLU
1	A	342	TYR
1	A	610	GLU
1	A	730	LYS
1	A	797	ARG
1	A	934	LEU
1	B	342	TYR
1	B	730	LYS
1	B	934	LEU
1	B	949	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	B	440	HIS
1	B	504	ASN
1	B	667	ASN
1	B	685	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 for Mogul analysis.

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
6	A1AUG	A	2105	-	6,8,8	1.11	0	6,9,9	1.95	2 (33%)
7	FMT	A	2106	-	2,2,2	0.44	0	1,1,1	0.39	0
2	NAD	A	2101	8	46,48,48	1.86	9 (19%)	64,73,73	1.63	13 (20%)
9	SO4	B	2207	-	4,4,4	0.38	0	6,6,6	0.13	0
3	FDA	B	2201	-	57,58,58	2.55	17 (29%)	78,89,89	1.83	18 (23%)
4	PGE	A	2103	-	9,9,9	0.32	0	8,8,8	0.46	0
6	A1AUG	B	2203	-	6,8,8	0.85	0	6,9,9	1.79	2 (33%)
9	SO4	A	2110	-	4,4,4	0.19	0	6,6,6	0.32	0
9	SO4	A	2111	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FMT	B	2204	-	2,2,2	0.91	0	1,1,1	0.40	0
3	FDA	A	2102	-	57,58,58	2.48	17 (29%)	78,89,89	1.82	19 (24%)
2	NAD	B	2205[B]	8	46,48,48	2.43	11 (23%)	64,73,73	1.69	9 (14%)
9	SO4	A	2112	-	4,4,4	0.20	0	6,6,6	0.21	0
5	PEG	A	2104	-	6,6,6	0.21	0	5,5,5	0.13	0
9	SO4	A	2109	-	4,4,4	0.34	0	6,6,6	0.47	0
9	SO4	B	2208	-	4,4,4	0.23	0	6,6,6	0.09	0
2	NAD	B	2205[A]	8	46,48,48	2.24	10 (21%)	64,73,73	1.68	11 (17%)
4	PGE	B	2202	-	9,9,9	0.30	0	8,8,8	0.57	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
6	A1AUG	A	2105	-	-	2/8/8/8	-
2	NAD	A	2101	8	-	3/30/62/62	0/5/5/5
3	FDA	B	2201	-	-	4/34/50/50	0/6/6/6
4	PGE	A	2103	-	-	3/7/7/7	-
6	A1AUG	B	2203	-	-	1/8/8/8	-
3	FDA	A	2102	-	-	5/34/50/50	0/6/6/6
2	NAD	B	2205[B]	8	-	6/30/62/62	0/5/5/5
5	PEG	A	2104	-	-	1/4/4/4	-
2	NAD	B	2205[A]	8	-	4/30/62/62	0/5/5/5
4	PGE	B	2202	-	-	3/7/7/7	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2201	FDA	PA-O3P	-11.25	1.47	1.59
2	B	2205[B]	NAD	PA-O3	-10.39	1.48	1.59
3	A	2102	FDA	PA-O3P	-9.69	1.49	1.59
2	B	2205[A]	NAD	PA-O3	-9.39	1.49	1.59
3	A	2102	FDA	O4-C4	6.77	1.36	1.23
2	B	2205[B]	NAD	C2N-N1N	6.08	1.41	1.35
2	B	2205[B]	NAD	C7N-N7N	5.91	1.43	1.33
3	B	2201	FDA	O4-C4	5.64	1.34	1.23
2	A	2101	NAD	C2N-N1N	5.63	1.41	1.35
2	A	2101	NAD	PA-O3	-5.40	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2201	FDA	C6-C5X	5.12	1.47	1.39
3	A	2102	FDA	P-O3P	5.04	1.64	1.59
3	A	2102	FDA	C9-C9A	5.02	1.47	1.39
3	A	2102	FDA	C6-C5X	4.88	1.47	1.39
2	B	2205[A]	NAD	C2N-N1N	4.88	1.40	1.35
3	B	2201	FDA	O2-C2	4.73	1.33	1.23
2	B	2205[A]	NAD	C7N-N7N	4.68	1.41	1.33
3	B	2201	FDA	C5X-C9A	-4.16	1.36	1.40
2	A	2101	NAD	C7N-N7N	4.05	1.40	1.33
2	B	2205[B]	NAD	C6A-N6A	3.80	1.43	1.34
3	B	2201	FDA	C4X-N5	3.79	1.43	1.35
2	B	2205[A]	NAD	C6A-N6A	3.75	1.43	1.34
3	A	2102	FDA	O2-C2	3.56	1.30	1.23
3	A	2102	FDA	C6A-N6A	3.46	1.43	1.34
3	A	2102	FDA	C4X-N5	3.45	1.42	1.35
3	B	2201	FDA	C2-N1	3.44	1.43	1.37
3	B	2201	FDA	C9-C9A	3.33	1.45	1.39
2	A	2101	NAD	C6A-N6A	3.14	1.42	1.34
3	B	2201	FDA	PA-O2A	-3.13	1.40	1.55
2	B	2205[A]	NAD	C6N-N1N	3.11	1.42	1.35
3	B	2201	FDA	P-O3P	3.07	1.62	1.59
3	B	2201	FDA	C6A-N6A	2.98	1.41	1.34
3	A	2102	FDA	C5X-N5	2.87	1.44	1.39
2	B	2205[B]	NAD	C6N-N1N	2.87	1.41	1.35
3	A	2102	FDA	PA-O5B	-2.75	1.48	1.59
3	B	2201	FDA	C1'-C2'	-2.75	1.48	1.52
3	B	2201	FDA	C10-N1	2.73	1.42	1.37
2	A	2101	NAD	C6N-N1N	2.67	1.41	1.35
3	A	2102	FDA	C5X-C9A	-2.65	1.37	1.40
3	A	2102	FDA	C10-N1	2.62	1.41	1.37
2	B	2205[B]	NAD	PA-O2A	-2.59	1.43	1.55
2	B	2205[A]	NAD	PA-O5B	-2.56	1.49	1.59
3	B	2201	FDA	O3B-C3B	-2.48	1.36	1.43
2	A	2101	NAD	PA-O2A	-2.43	1.44	1.55
3	A	2102	FDA	O2'-C2'	-2.29	1.38	1.43
3	A	2102	FDA	C5A-C4A	2.28	1.43	1.39
3	A	2102	FDA	C2B-C3B	-2.27	1.47	1.53
2	B	2205[A]	NAD	O2D-C2D	-2.26	1.37	1.43
3	B	2201	FDA	O4'-C4'	-2.24	1.38	1.43
3	B	2201	FDA	C5X-N5	2.18	1.43	1.39
2	B	2205[A]	NAD	O2B-C2B	-2.17	1.37	1.43
2	B	2205[A]	NAD	O3D-C3D	-2.12	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2205[B]	NAD	O2B-C2B	-2.11	1.37	1.43
2	B	2205[B]	NAD	O3D-C3D	-2.11	1.37	1.43
2	B	2205[B]	NAD	C2D-C3D	-2.09	1.47	1.53
3	A	2102	FDA	C2-N1	2.08	1.40	1.37
2	A	2101	NAD	O2B-C2B	-2.07	1.37	1.43
3	B	2201	FDA	C2B-C3B	-2.07	1.47	1.53
2	A	2101	NAD	PA-O5B	-2.06	1.51	1.59
2	B	2205[B]	NAD	C2B-C3B	-2.06	1.47	1.53
2	A	2101	NAD	C2D-C3D	-2.05	1.47	1.53
2	B	2205[B]	NAD	PA-O5B	-2.02	1.51	1.59
3	A	2102	FDA	PA-O2A	-2.01	1.46	1.55
2	B	2205[A]	NAD	PA-O1A	2.00	1.57	1.50

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2101	NAD	N3A-C2A-N1A	-5.67	120.00	128.58
2	B	2205[B]	NAD	N3A-C2A-N1A	-5.66	120.01	128.58
2	B	2205[A]	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
3	A	2102	FDA	N3A-C2A-N1A	-5.21	120.70	128.58
2	B	2205[A]	NAD	C5A-C4A-N3A	-4.97	119.88	126.72
3	A	2102	FDA	C5A-C4A-N3A	-4.92	119.95	126.72
2	B	2205[B]	NAD	C5A-C4A-N3A	-4.69	120.26	126.72
3	B	2201	FDA	N3A-C2A-N1A	-4.58	121.65	128.58
3	B	2201	FDA	N3-C2-N1	4.48	122.78	115.74
3	A	2102	FDA	N3A-C4A-N9A	4.43	134.70	127.17
3	A	2102	FDA	C4-N3-C2	-4.32	120.42	126.37
3	B	2201	FDA	C4-N3-C2	-4.28	120.47	126.37
3	B	2201	FDA	C5A-C4A-N3A	-4.18	120.96	126.72
3	A	2102	FDA	C5A-N7A-C8A	4.05	109.81	103.45
3	B	2201	FDA	C9-C9A-N10	-3.94	116.56	121.85
2	B	2205[A]	NAD	N3A-C4A-N9A	3.89	133.78	127.17
3	A	2102	FDA	N9A-C8A-N7A	-3.85	108.47	113.94
2	B	2205[A]	NAD	C2A-N3A-C4A	3.75	120.99	111.83
2	A	2101	NAD	C5A-C4A-N3A	-3.71	121.60	126.72
2	B	2205[B]	NAD	N3A-C4A-N9A	3.68	133.43	127.17
2	A	2101	NAD	C2N-C3N-C4N	3.63	122.48	118.26
2	B	2205[B]	NAD	C2A-N3A-C4A	3.63	120.69	111.83
2	B	2205[A]	NAD	C5A-N7A-C8A	3.61	109.12	103.45
3	B	2201	FDA	O2A-PA-O3P	-3.58	97.59	107.27
3	A	2102	FDA	N3-C2-N1	3.56	121.33	115.74
6	A	2105	A1AUG	CB-CG-CD	-3.55	102.30	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2205[B]	NAD	C5A-N7A-C8A	3.55	109.02	103.45
2	A	2101	NAD	C5A-N7A-C8A	3.48	108.92	103.45
2	A	2101	NAD	N3A-C4A-N9A	3.40	132.96	127.17
3	B	2201	FDA	C5A-N7A-C8A	3.40	108.79	103.45
3	A	2102	FDA	C4A-N9A-C8A	3.38	109.29	105.74
3	A	2102	FDA	C2A-N3A-C4A	3.38	120.08	111.83
2	B	2205[B]	NAD	C6N-N1N-C2N	-3.30	119.07	121.88
3	B	2201	FDA	N3A-C4A-N9A	3.26	132.70	127.17
2	A	2101	NAD	C4D-O4D-C1D	-3.23	106.96	109.92
2	B	2205[A]	NAD	C2N-C3N-C4N	3.22	122.01	118.26
3	B	2201	FDA	C5X-C9A-N10	3.21	121.65	118.01
3	A	2102	FDA	C4A-C5A-N7A	-3.07	107.07	110.58
3	B	2201	FDA	C4A-C5A-N7A	-3.00	107.15	110.58
2	B	2205[A]	NAD	N9A-C8A-N7A	-3.00	109.68	113.94
2	B	2205[B]	NAD	N9A-C8A-N7A	-3.00	109.68	113.94
2	A	2101	NAD	C2A-N3A-C4A	2.93	118.99	111.83
6	B	2203	A1AUG	CG-CB-CA	-2.80	106.25	115.24
3	B	2201	FDA	O2P-P-O3P	2.80	114.83	107.27
3	B	2201	FDA	C2A-N3A-C4A	2.78	118.63	111.83
3	B	2201	FDA	O3P-PA-O1A	2.76	119.02	110.70
3	B	2201	FDA	C5X-N5-C4X	-2.74	114.75	121.08
2	B	2205[B]	NAD	C4A-C5A-N7A	-2.70	107.49	110.58
2	B	2205[A]	NAD	C4A-C5A-N7A	-2.70	107.50	110.58
2	A	2101	NAD	C4A-C5A-N7A	-2.69	107.51	110.58
3	A	2102	FDA	C9A-C5X-N5	2.57	122.50	119.37
3	B	2201	FDA	N9A-C8A-N7A	-2.54	110.33	113.94
2	A	2101	NAD	N9A-C8A-N7A	-2.53	110.34	113.94
2	A	2101	NAD	C2A-N1A-C6A	2.48	122.80	118.73
2	A	2101	NAD	C5N-C4N-C3N	-2.44	117.97	120.36
3	A	2102	FDA	C9-C9A-N10	-2.41	118.61	121.85
3	A	2102	FDA	O2-C2-N3	-2.41	117.58	121.86
6	B	2203	A1AUG	CB-CG-CD	-2.40	105.52	112.27
3	A	2102	FDA	O2A-PA-O3P	-2.37	100.87	107.27
3	A	2102	FDA	C4X-C4-N3	2.32	118.51	112.13
2	B	2205[B]	NAD	C2N-C3N-C4N	2.27	120.90	118.26
3	B	2201	FDA	C4X-C4-N3	2.26	118.34	112.13
3	A	2102	FDA	C4-C4X-N5	2.10	121.73	116.37
6	A	2105	A1AUG	CG-CB-CA	-2.07	108.61	115.24
3	A	2102	FDA	C5X-N5-C4X	-2.05	116.34	121.08
2	A	2101	NAD	O5B-PA-O1A	2.05	117.06	108.94
2	B	2205[A]	NAD	O2A-PA-O5B	-2.04	98.32	107.57
3	B	2201	FDA	C1'-N10-C9A	2.04	124.59	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2102	FDA	O4-C4-C4X	-2.03	122.36	127.26
2	B	2205[A]	NAD	C6N-N1N-C2N	-2.03	120.15	121.88
3	B	2201	FDA	O2-C2-N3	-2.02	118.28	121.86
2	A	2101	NAD	C6N-N1N-C2N	-2.01	120.16	121.88
3	A	2102	FDA	C9-C9A-C5X	2.01	122.76	119.95
2	B	2205[A]	NAD	C5A-C6A-N6A	-2.00	118.33	123.29

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2105	A1AUG	CA-CB-CG-CD
6	A	2105	A1AUG	OE1-CD-CG-CB
6	B	2203	A1AUG	CA-CB-CG-CD
3	A	2102	FDA	C2'-C3'-C4'-O4'
4	A	2103	PGE	O3-C5-C6-O4
4	B	2202	PGE	O1-C1-C2-O2
2	B	2205[B]	NAD	PN-O3-PA-O1A
2	B	2205[A]	NAD	PN-O3-PA-O5B
2	B	2205[A]	NAD	C4D-C5D-O5D-PN
2	A	2101	NAD	C2B-C1B-N9A-C8A
2	B	2205[A]	NAD	C2B-C1B-N9A-C8A
2	B	2205[B]	NAD	PA-O3-PN-O2N
3	A	2102	FDA	PA-O3P-P-O1P
2	A	2101	NAD	C4D-C5D-O5D-PN
4	B	2202	PGE	C4-C3-O2-C2
2	B	2205[B]	NAD	C2B-C1B-N9A-C8A
4	A	2103	PGE	O2-C3-C4-O3
4	A	2103	PGE	C3-C4-O3-C5
2	B	2205[B]	NAD	PN-O3-PA-O2A
3	B	2201	FDA	C2'-C3'-C4'-O4'
3	A	2102	FDA	O3'-C3'-C4'-O4'
3	B	2201	FDA	C4'-C5'-O5'-P
2	B	2205[B]	NAD	O4B-C1B-N9A-C8A
3	A	2102	FDA	C2'-C3'-C4'-C5'
4	B	2202	PGE	O3-C5-C6-O4
2	B	2205[A]	NAD	O4B-C1B-N9A-C8A
2	B	2205[B]	NAD	PA-O3-PN-O1N
3	A	2102	FDA	PA-O3P-P-O2P
2	A	2101	NAD	O4B-C1B-N9A-C8A
3	B	2201	FDA	O3'-C3'-C4'-C5'
3	B	2201	FDA	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
5	A	2104	PEG	C4-C3-O2-C2

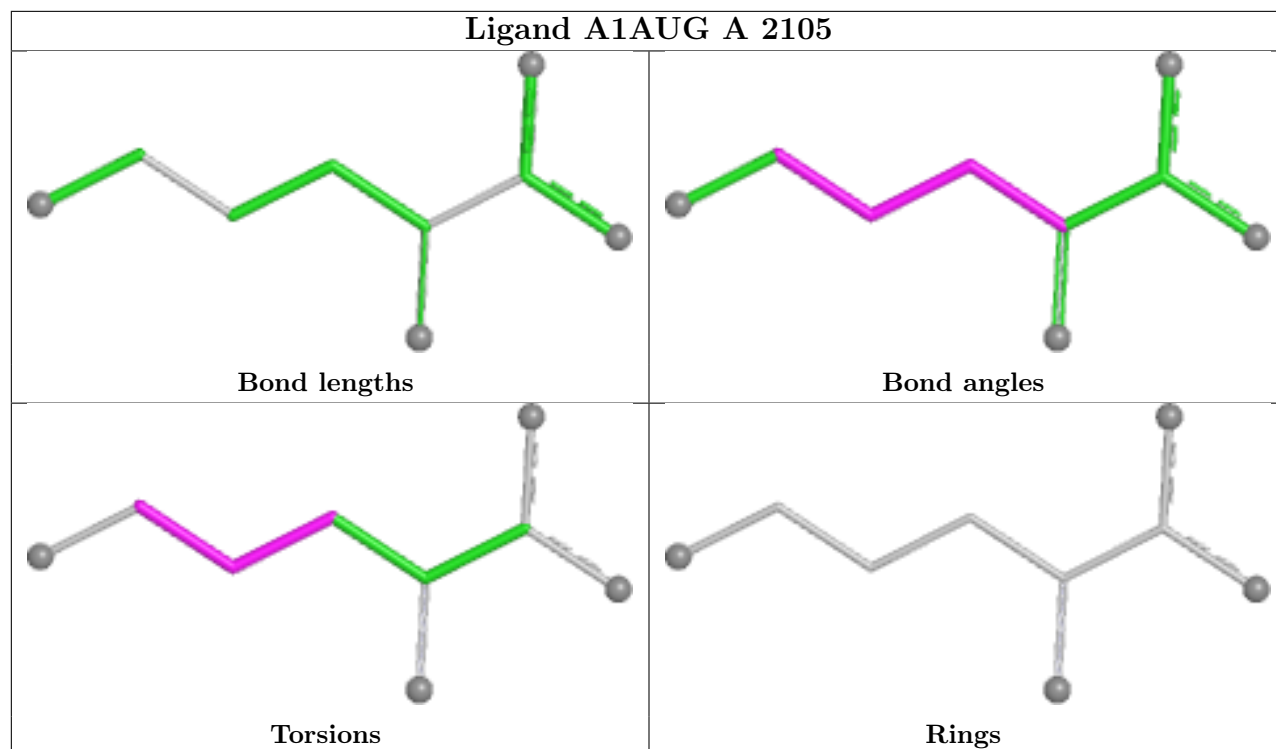
There are no ring outliers.

6 monomers are involved in 9 short contacts:

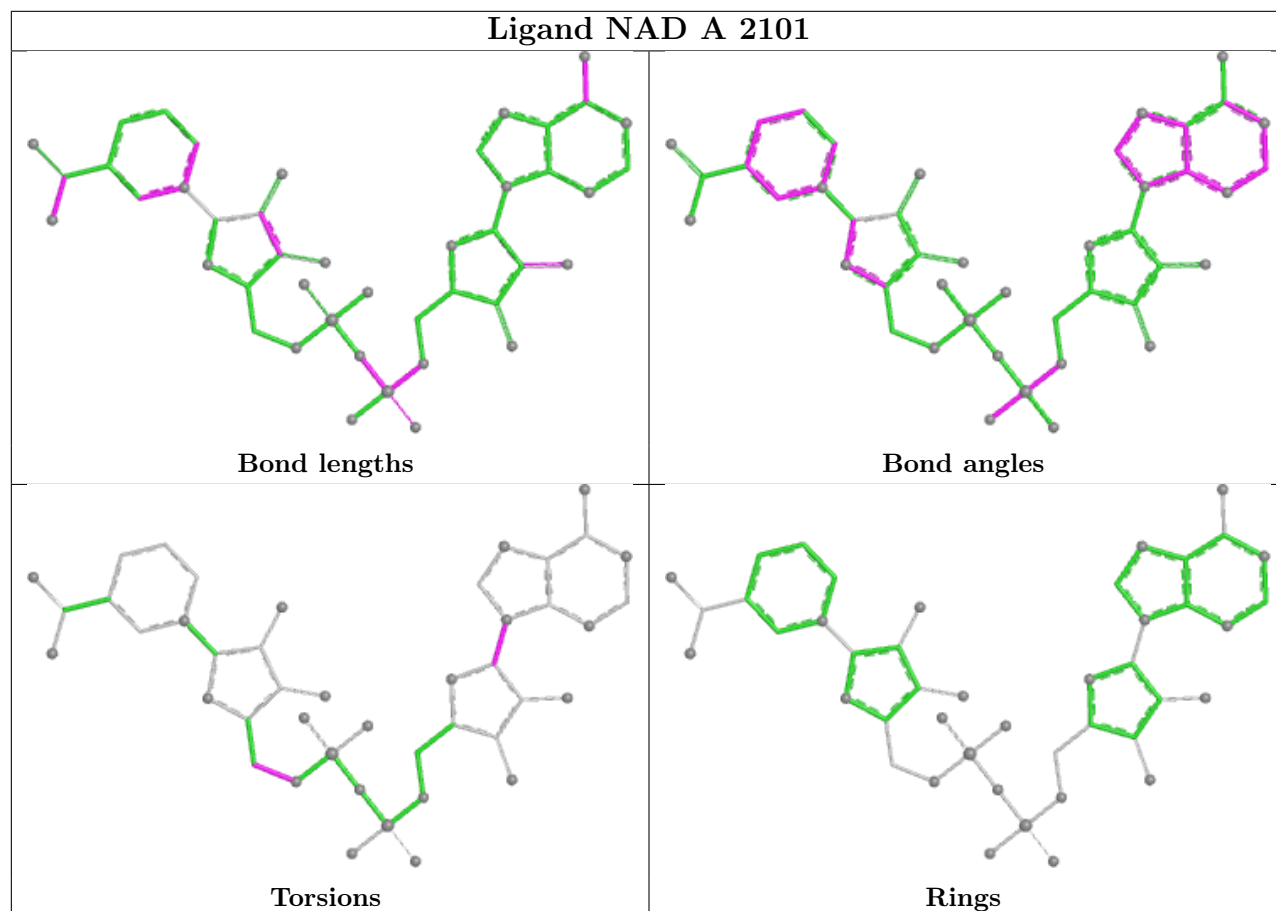
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2105	A1AUG	1	0
3	B	2201	FDA	1	0
6	B	2203	A1AUG	2	0
3	A	2102	FDA	3	0
2	B	2205[B]	NAD	2	0
2	B	2205[A]	NAD	1	0

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.

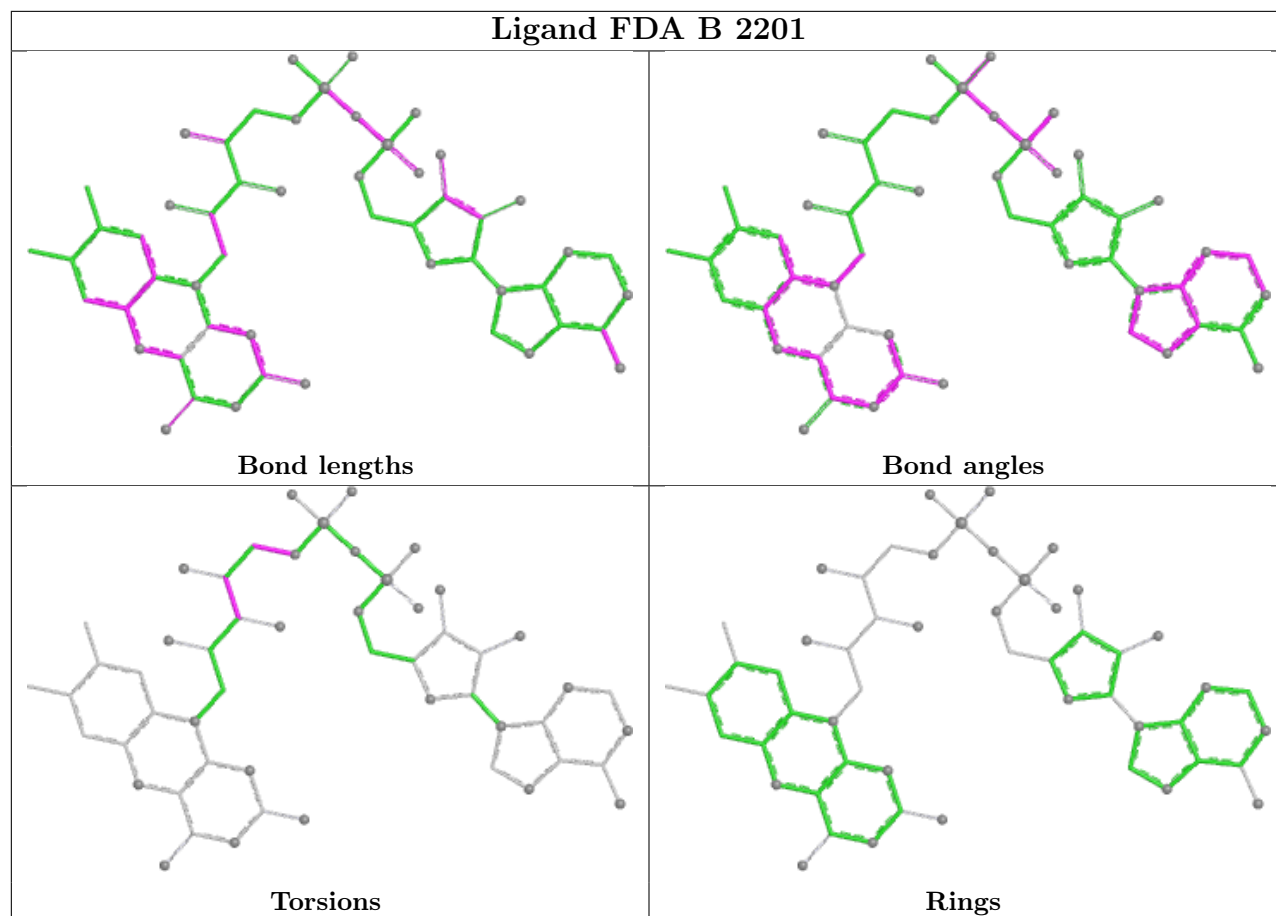
Ligand A1AUG A 2105



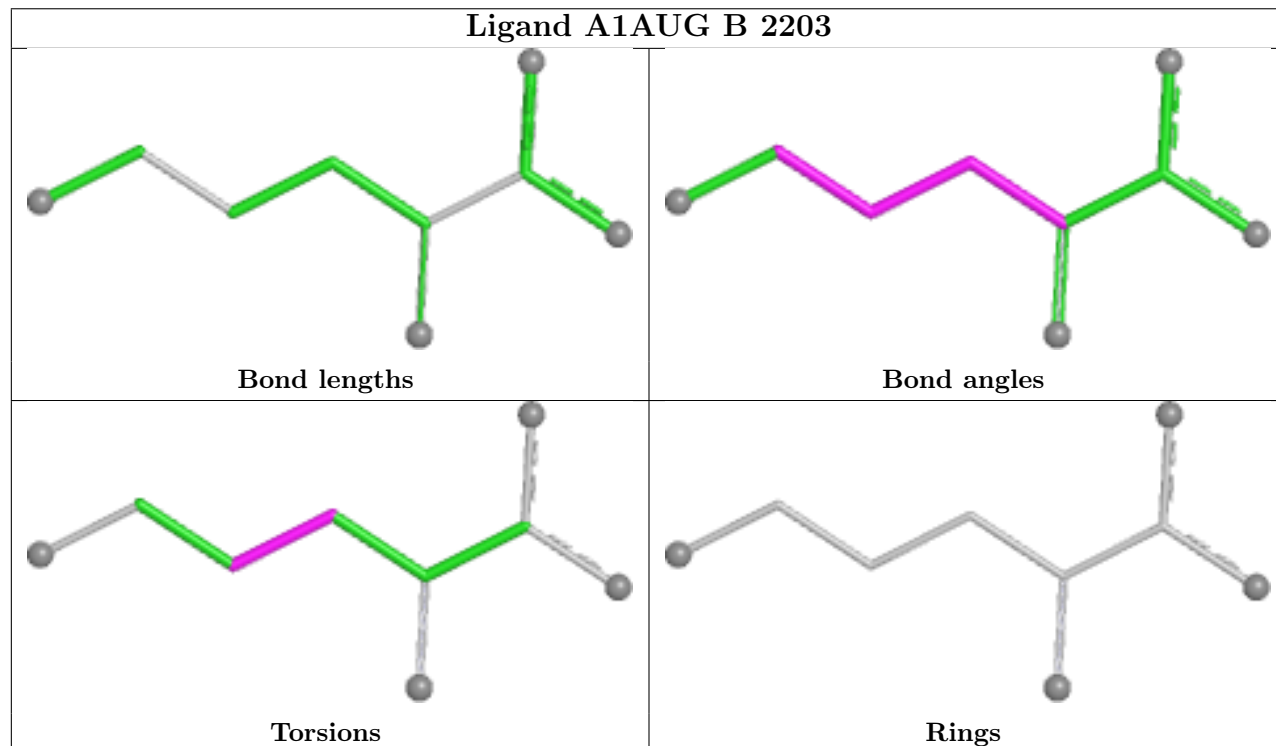
Ligand NAD A 2101

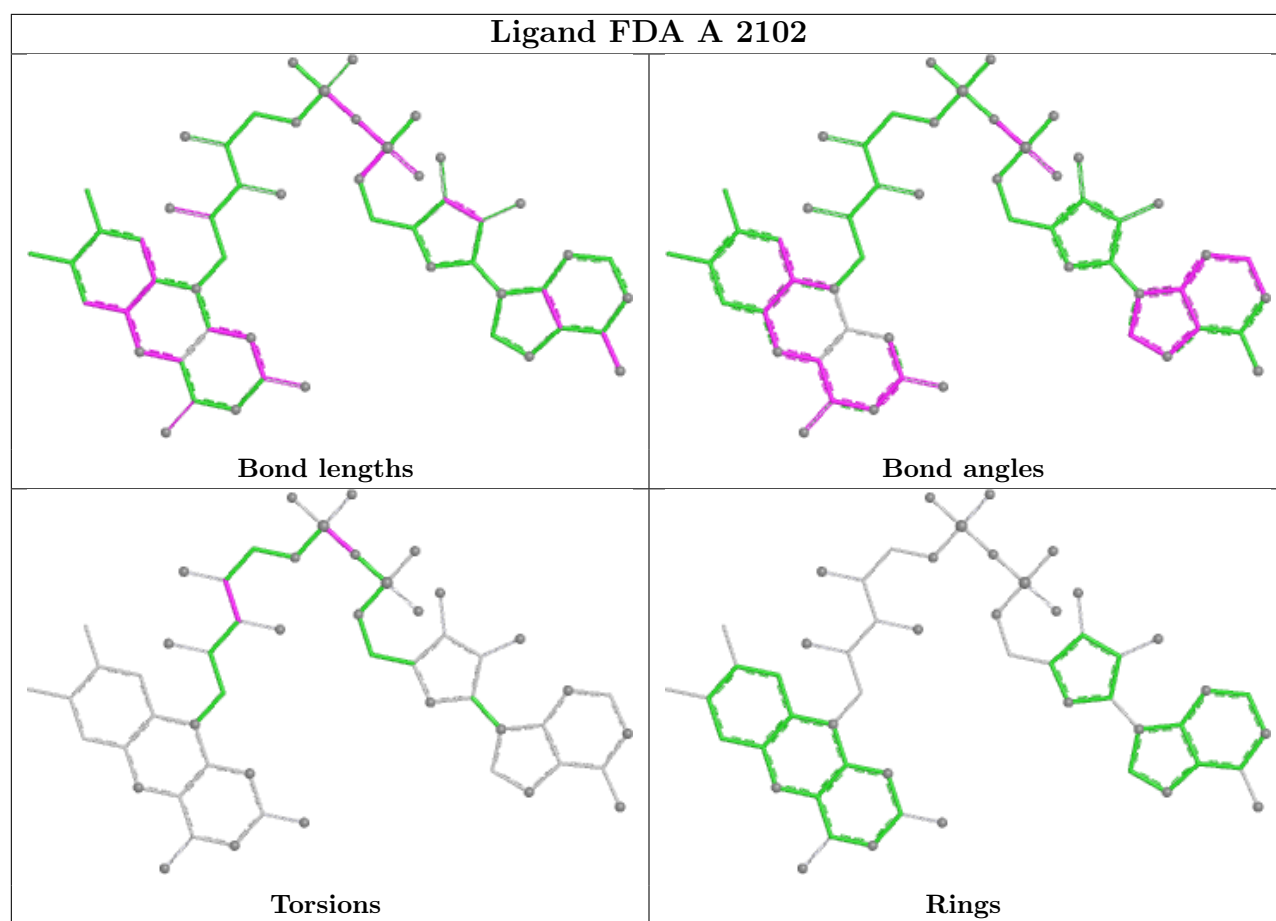


Ligand FDA B 2201

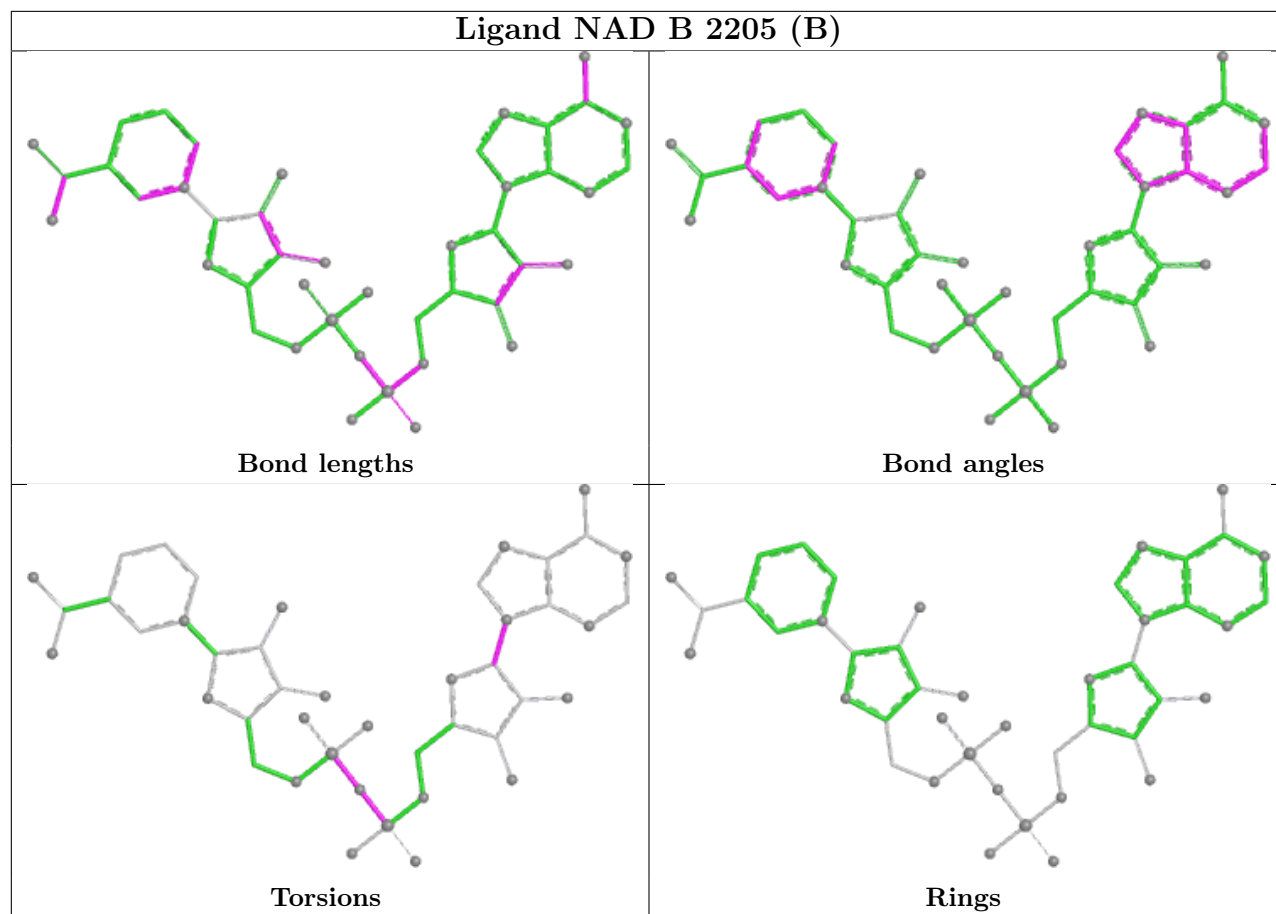


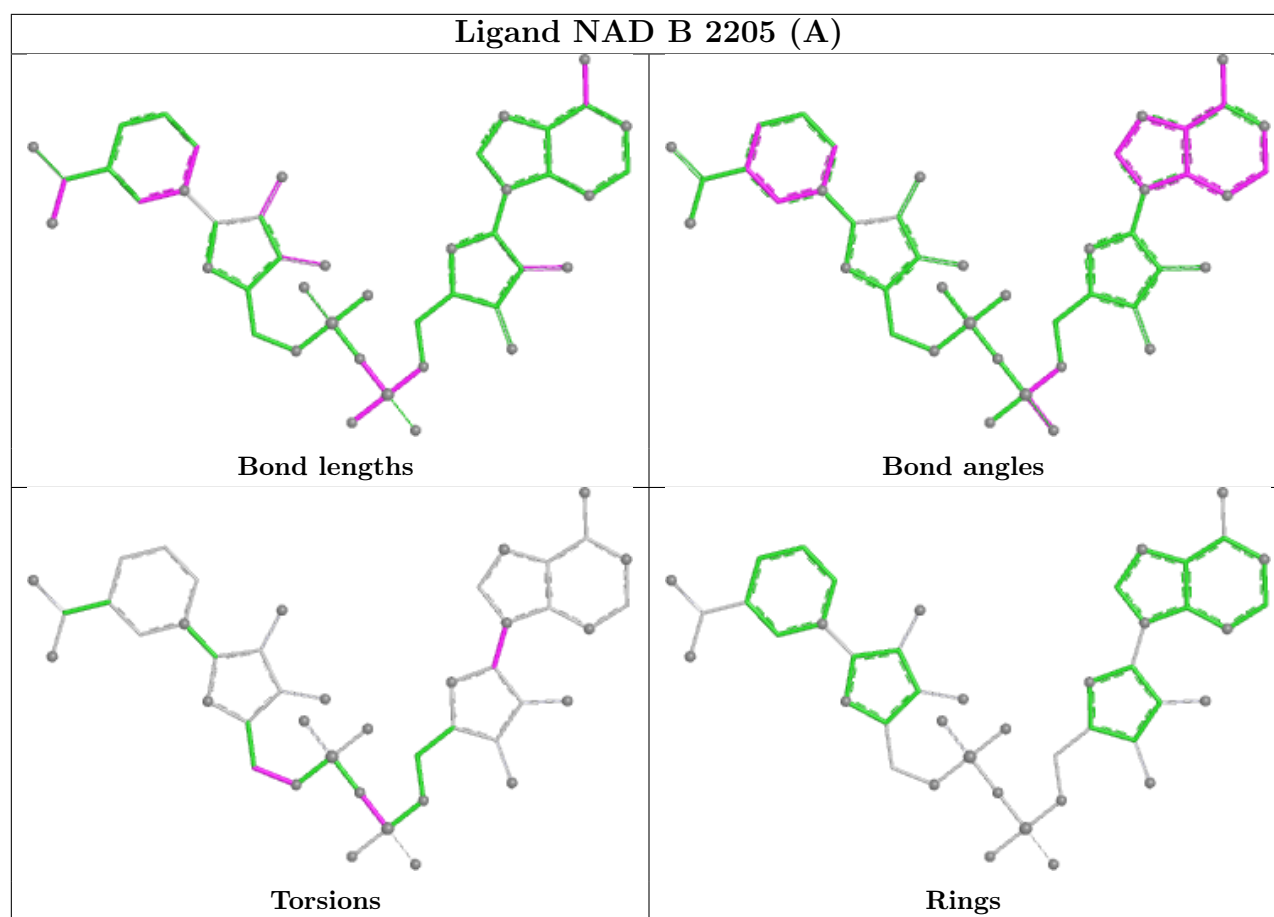
Ligand A1AUG B 2203





Ligand NAD B 2205 (B)





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	1210/1235 (97%)	-0.01	54 (4%)	38	42	8, 22, 43, 69	6 (0%)
1	B	1209/1235 (97%)	0.08	70 (5%)	29	31	7, 21, 43, 65	8 (0%)
All	All	2419/2470 (97%)	0.04	124 (5%)	33	36	7, 21, 43, 69	14 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	TYR	6.5
1	A	485	TYR	5.7
1	A	493	ASN	5.7
1	B	1227	ALA	5.3
1	A	224	GLY	5.3
1	B	482	LEU	5.2
1	B	481	THR	4.9
1	A	132	SER	4.7
1	B	83	GLY	4.5
1	A	137	SER	4.4
1	A	129	ASN	4.2
1	B	508	VAL	4.2
1	A	490	LEU	4.2
1	B	484	ALA	4.2
1	B	912	ILE	4.1
1	A	127	ASP	4.1
1	B	514	ILE	4.1
1	B	132	SER	4.1
1	A	492	GLU	4.0
1	B	497	SER	4.0
1	A	491	LEU	4.0
1	A	482	LEU	4.0
1	B	487	VAL	3.9
1	A	83	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	506	PRO	3.7
1	A	486	LEU	3.7
1	A	495	ALA	3.7
1	B	503	ILE	3.6
1	A	496	ASN	3.6
1	B	488	ARG	3.6
1	B	115	ALA	3.6
1	A	484	ALA	3.5
1	B	134	LEU	3.4
1	B	486	LEU	3.4
1	A	134	LEU	3.3
1	B	127	ASP	3.3
1	B	462	GLY	3.3
1	B	1230	MET	3.2
1	A	115	ALA	3.2
1	B	1229	LEU	3.2
1	A	125	ILE	3.2
1	A	483	LEU	3.1
1	A	1227	ALA	3.1
1	B	495	ALA	3.1
1	A	1002[A]	GLY	3.0
1	B	490	LEU	3.0
1	B	439	PHE	3.0
1	B	116	THR	3.0
1	B	14	ALA	3.0
1	B	494	GLY	2.9
1	B	801	ALA	2.9
1	B	510	ILE	2.9
1	A	494	GLY	2.9
1	B	1228	SER	2.9
1	A	14	ALA	2.8
1	B	1058	ASP	2.8
1	B	440	HIS	2.8
1	B	478	THR	2.7
1	B	129	ASN	2.7
1	B	913	GLY	2.7
1	B	223	LEU	2.7
1	B	463	ARG	2.7
1	B	464	GLY	2.7
1	A	130	TRP	2.7
1	A	506	PRO	2.6
1	B	133	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	796	ASP	2.6
1	A	112	PRO	2.6
1	B	128	GLY	2.6
1	A	195	PHE	2.6
1	A	131	LYS	2.6
1	A	133	HIS	2.6
1	A	111	ILE	2.5
1	A	225	GLU	2.5
1	A	508	VAL	2.5
1	B	414	ASP	2.5
1	B	800	PRO	2.4
1	A	113	ASP	2.4
1	A	523	ALA	2.4
1	B	1223	ALA	2.4
1	B	78	LYS	2.4
1	A	120	LEU	2.4
1	B	149	LEU	2.4
1	B	456	LEU	2.4
1	B	1063	ARG	2.4
1	A	192	GLY	2.4
1	A	1003[A]	ALA	2.3
1	A	489	ARG	2.3
1	A	801	ALA	2.3
1	A	114	THR	2.3
1	A	156	THR	2.3
1	B	498	SER	2.3
1	A	937	LEU	2.2
1	B	496	ASN	2.2
1	A	226	ALA	2.2
1	A	1222	ALA	2.2
1	B	1222	ALA	2.2
1	B	225	GLU	2.2
1	B	451	GLY	2.2
1	B	415	VAL	2.2
1	B	114	THR	2.2
1	B	437	LYS	2.2
1	B	507	LYS	2.2
1	B	491	LEU	2.1
1	B	937	LEU	2.1
1	A	938	GLN	2.1
1	B	904	GLY	2.1
1	A	773	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	492	GLU	2.1
1	B	479	HIS	2.1
1	A	128	GLY	2.1
1	B	480	GLU	2.1
1	B	499	PHE	2.1
1	A	75	LEU	2.1
1	B	138	ARG	2.1
1	A	481	THR	2.0
1	B	523	ALA	2.0
1	A	503	ILE	2.0
1	B	509	SER	2.0
1	A	571	ALA	2.0
1	B	74	ALA	2.0
1	B	483	LEU	2.0
1	B	66	SER	2.0
1	A	504	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

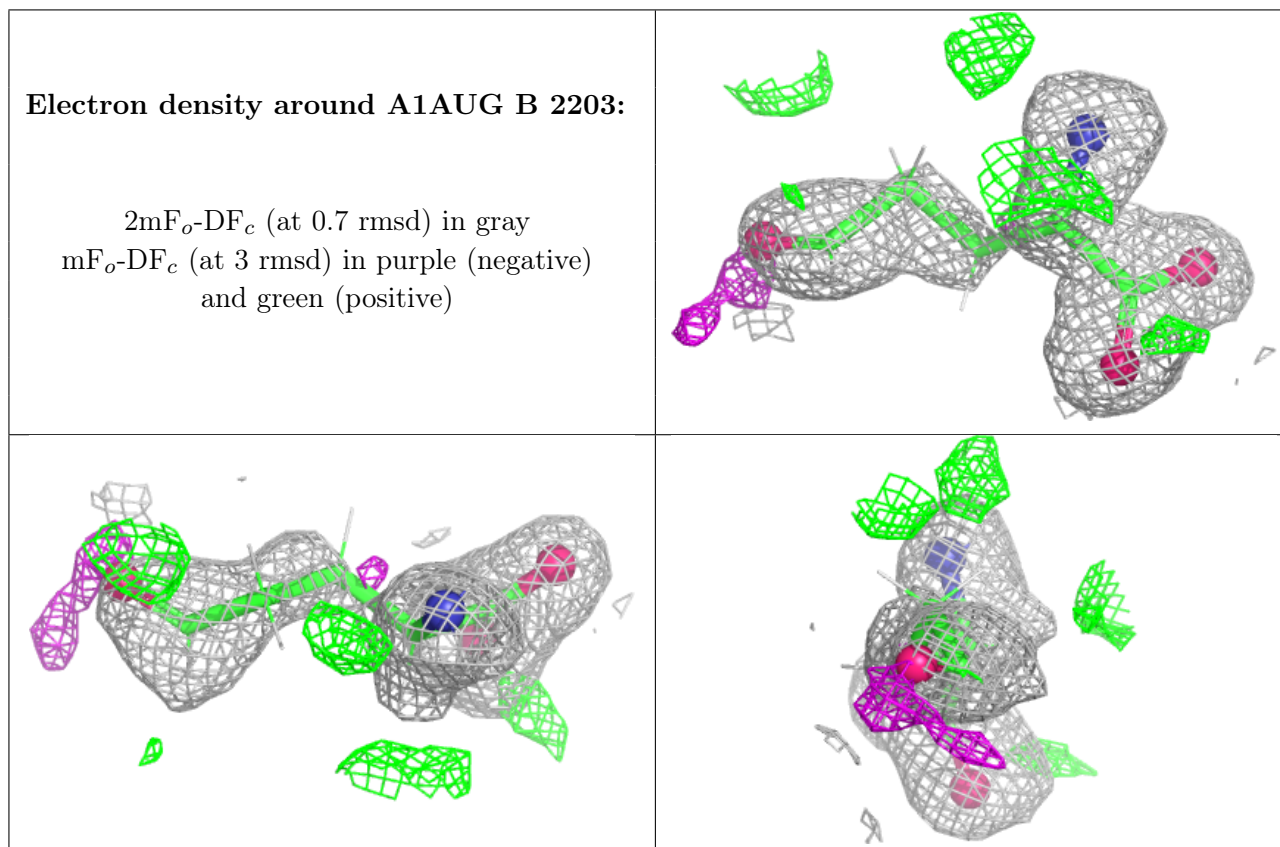
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SO4	B	2208	5/5	0.81	0.13	43,48,53,53	5
9	SO4	A	2111	5/5	0.89	0.09	50,53,56,57	0
4	PGE	A	2103	10/10	0.90	0.10	23,32,46,55	0
6	A1AUG	B	2203	9/9	0.90	0.14	8,23,28,28	17
6	A1AUG	A	2105	9/9	0.91	0.14	6,25,34,34	17
9	SO4	A	2110	5/5	0.91	0.11	33,34,43,45	5
5	PEG	A	2104	7/7	0.92	0.08	26,32,40,42	0

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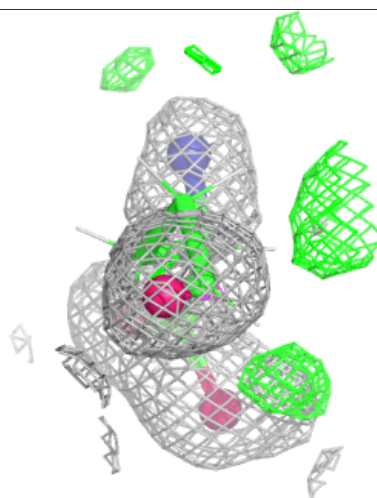
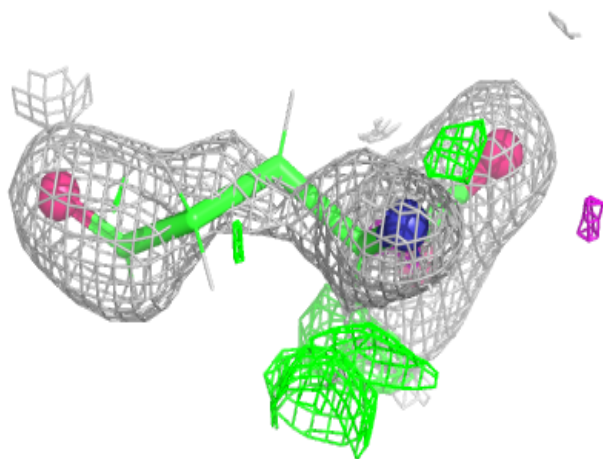
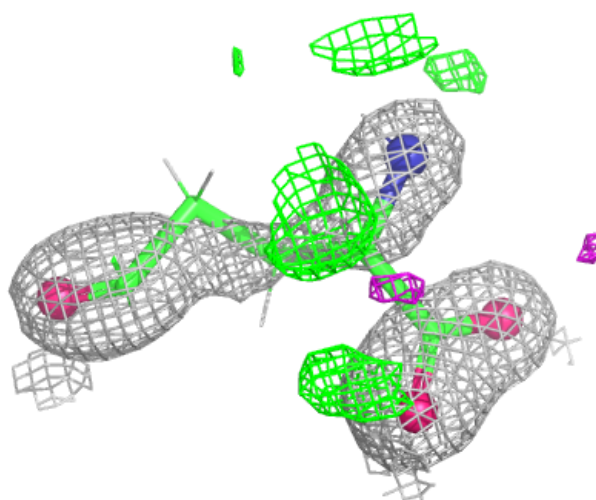
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGE	B	2202	10/10	0.93	0.09	23,34,45,48	0
9	SO4	A	2112	5/5	0.94	0.10	24,26,35,44	5
7	FMT	A	2106	3/3	0.95	0.10	15,18,29,30	0
2	NAD	B	2205[B]	44/44	0.96	0.07	12,16,21,22	70
7	FMT	B	2204	3/3	0.96	0.10	11,13,28,32	0
2	NAD	B	2205[A]	44/44	0.96	0.07	7,15,19,22	70
3	FDA	B	2201	53/53	0.97	0.06	13,19,27,32	0
2	NAD	A	2101	44/44	0.97	0.06	14,18,23,28	0
3	FDA	A	2102	53/53	0.97	0.06	12,19,27,30	0
9	SO4	A	2109	5/5	0.99	0.03	15,16,17,18	0
8	MG	A	2107	1/1	0.99	0.05	22,22,22,22	0
8	MG	A	2108	1/1	0.99	0.12	23,23,23,23	0
8	MG	B	2206[A]	1/1	0.99	0.02	13,13,13,13	1
9	SO4	B	2207	5/5	0.99	0.04	13,15,18,19	0
8	MG	B	2206[B]	1/1	0.99	0.02	20,20,20,20	1

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.



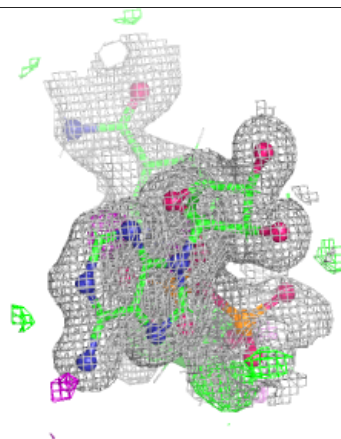
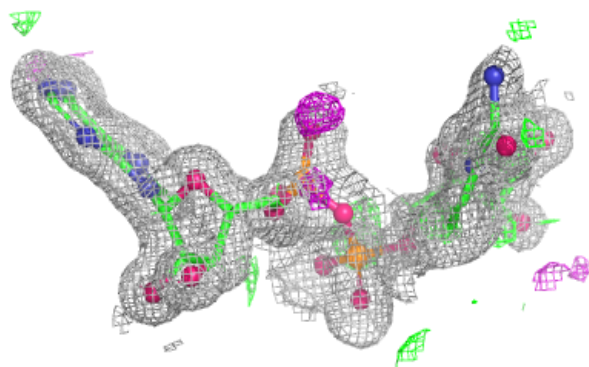
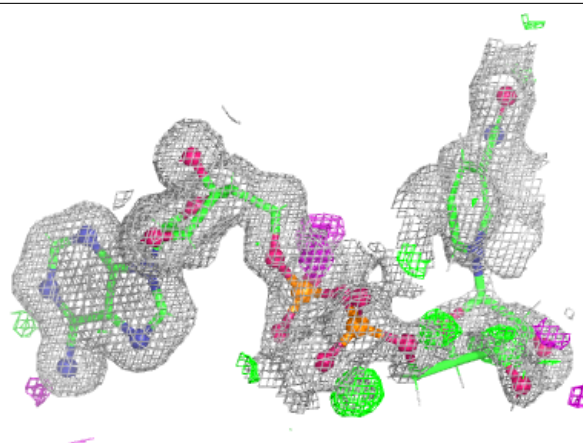
Electron density around A1AUG A 2105:

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



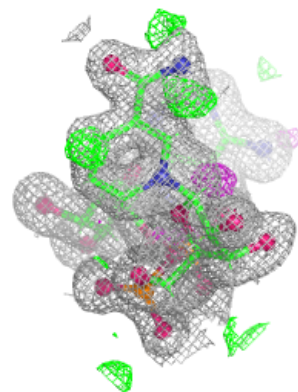
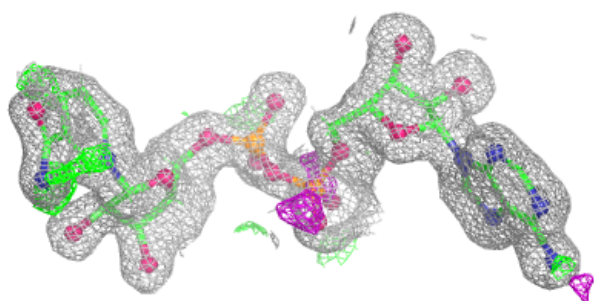
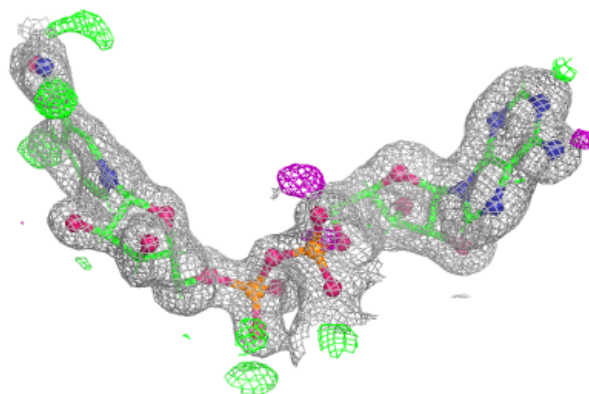
Electron density around NAD B 2205 (B):

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

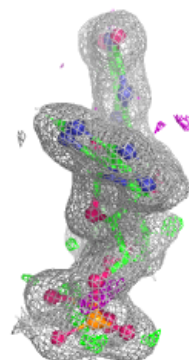
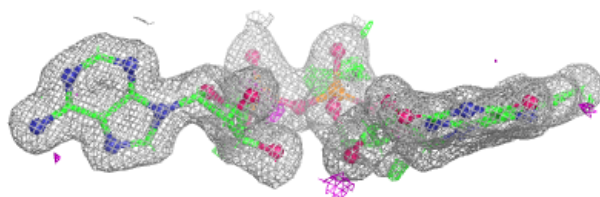
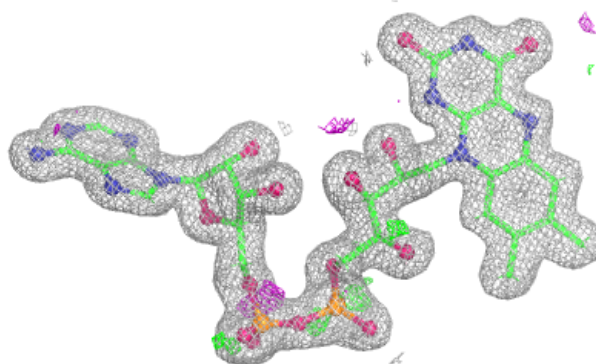


Electron density around NAD B 2205 (A):

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

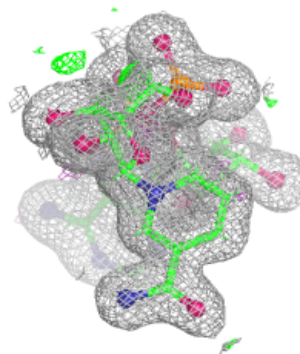
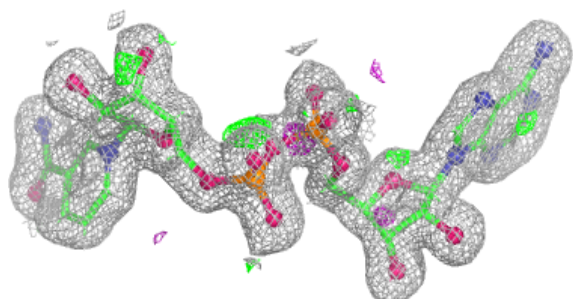
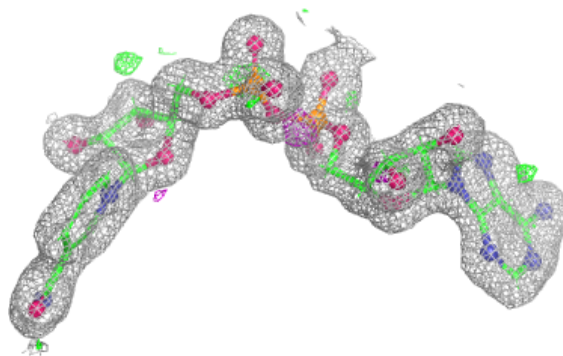
**Electron density around FDA B 2201:**

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

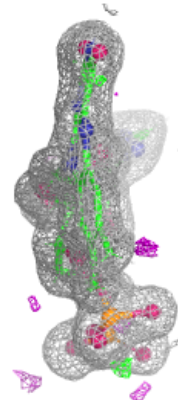
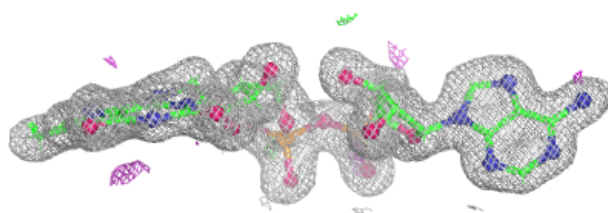
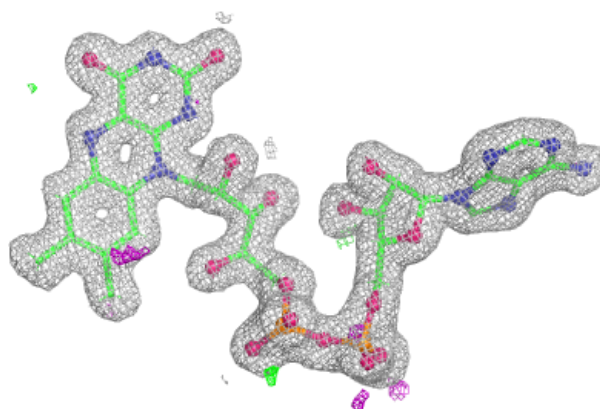


Electron density around NAD A 2101:

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

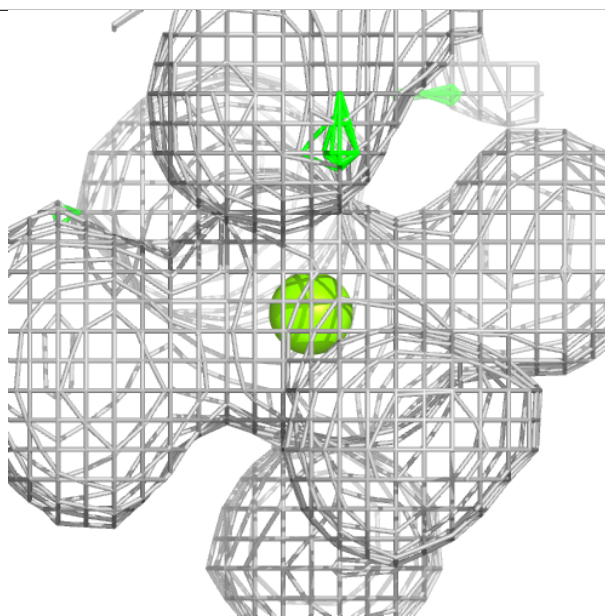
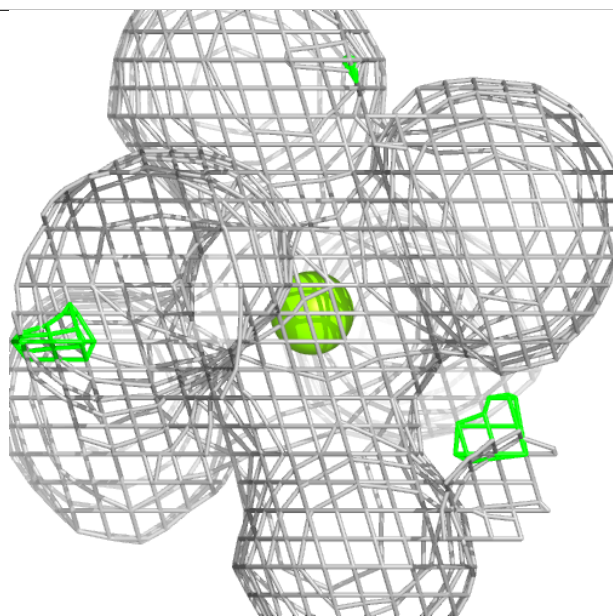
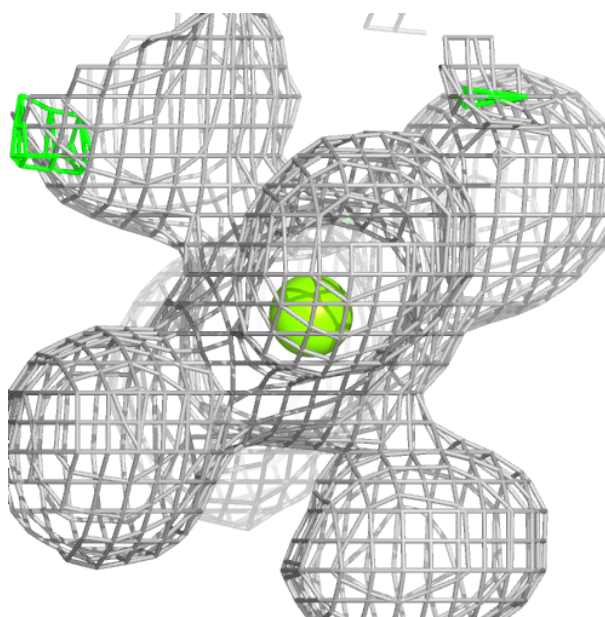
**Electron density around FDA A 2102:**

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



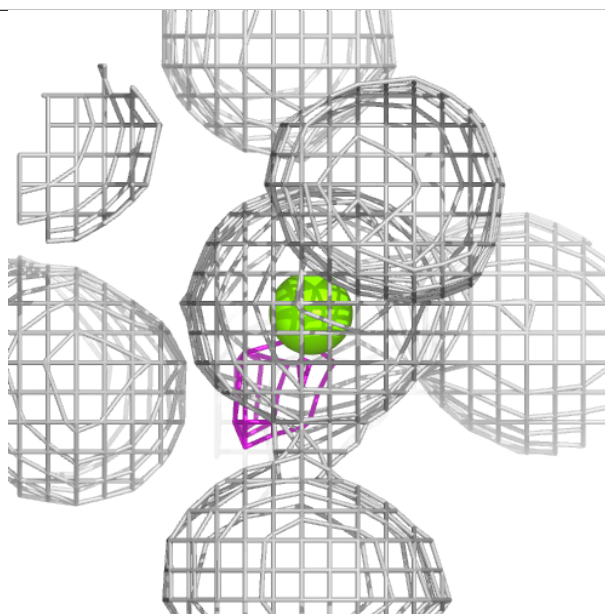
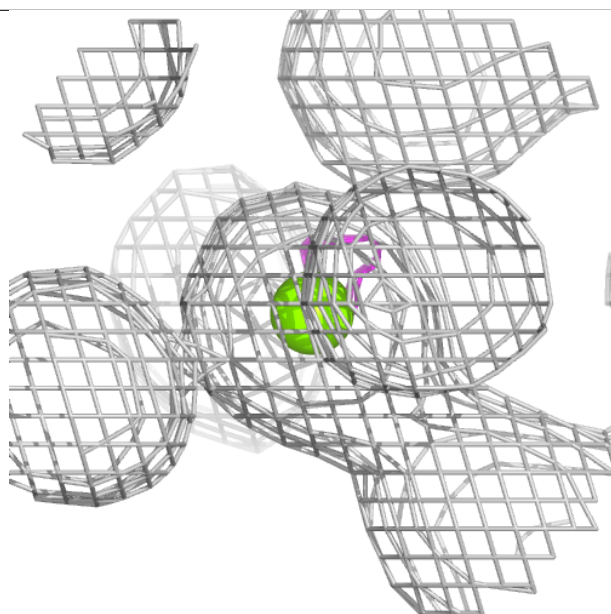
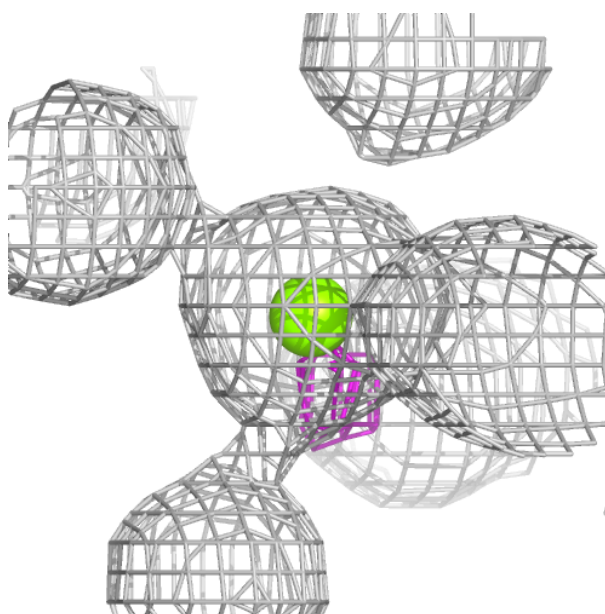
Electron density around MG A 2107:

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



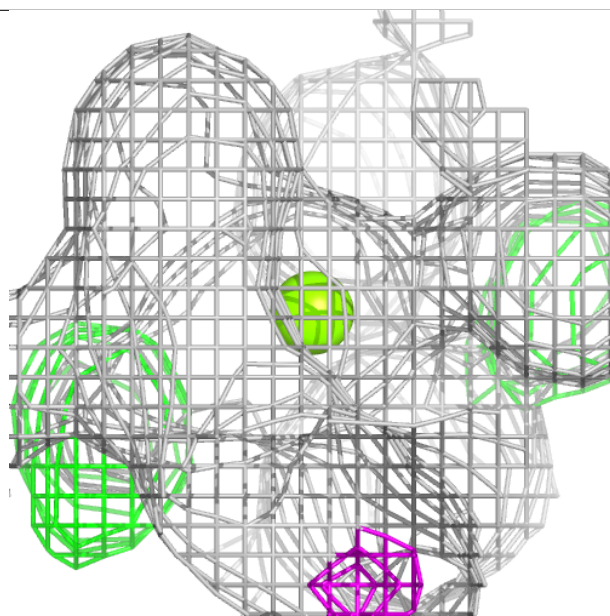
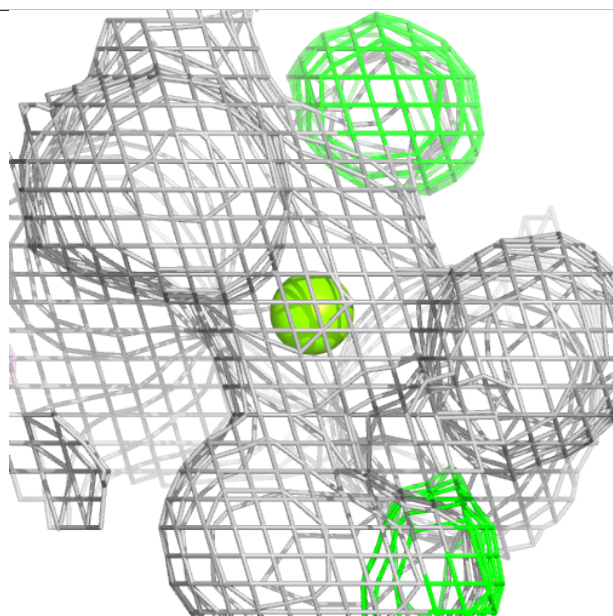
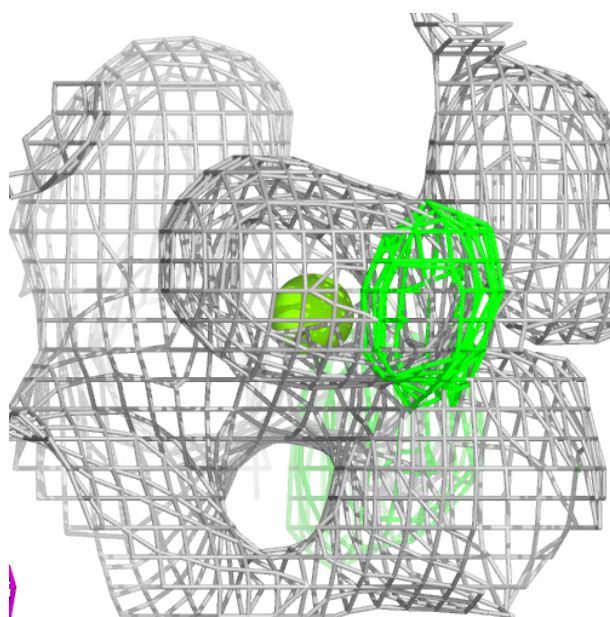
Electron density around MG A 2108:

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



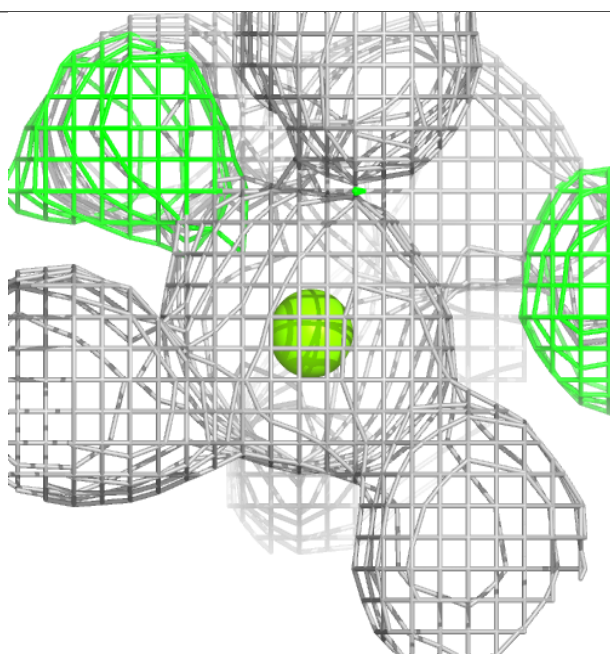
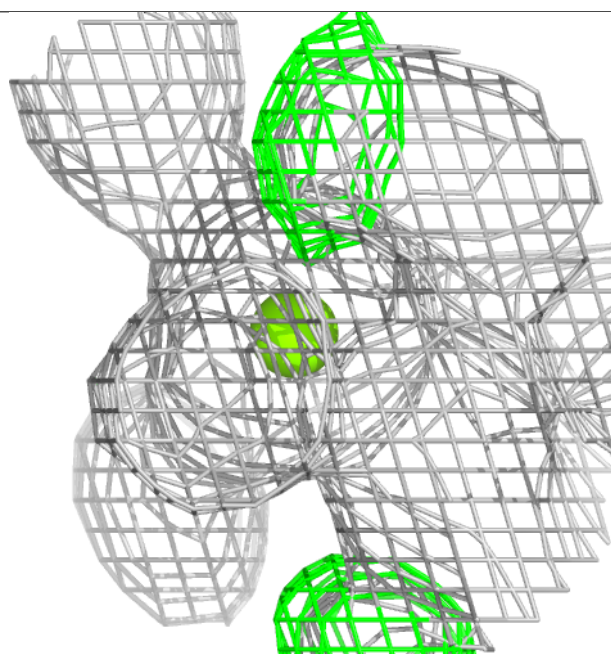
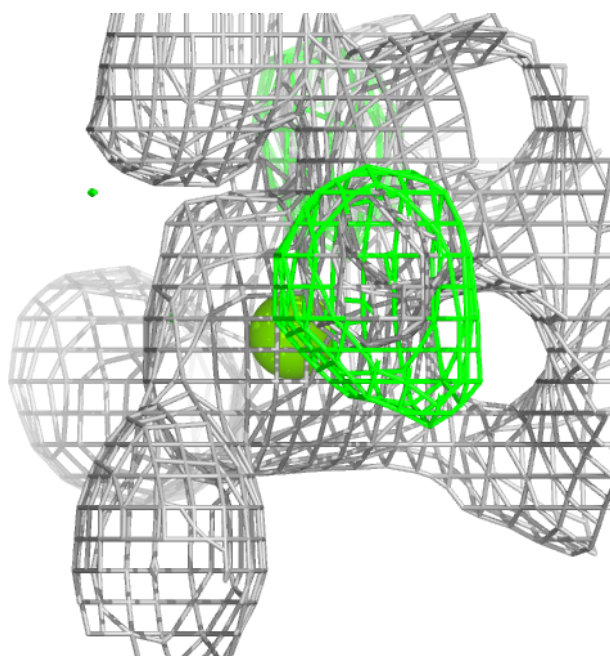
Electron density around MG B 2206 (A):

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



Electron density around MG B 2206 (B):

$2mF_o-DF_c$ (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.