



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 11:06 AM EDT

PDB ID : 9C34 / pdb_00009c34
Title : Proline utilization A with the FADH- N5 atom covalently modified by proline
Authors : Tanner, J.J.; Buckley, D.P.
Deposited on : 2024-05-31
Resolution : 1.88 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

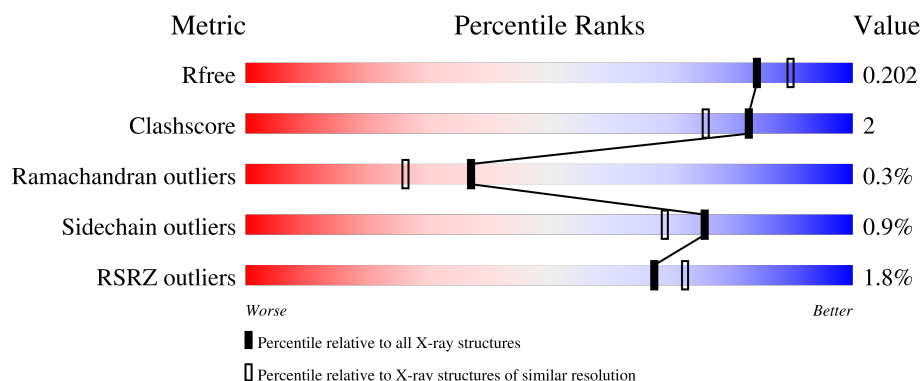
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

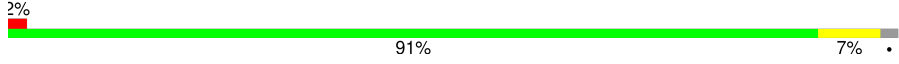
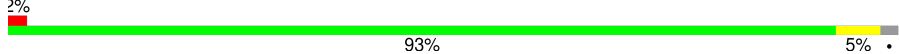
The reported resolution of this entry is 1.88 Å.

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}	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	
1	B	1235	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 36865 atoms, of which 17657 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.

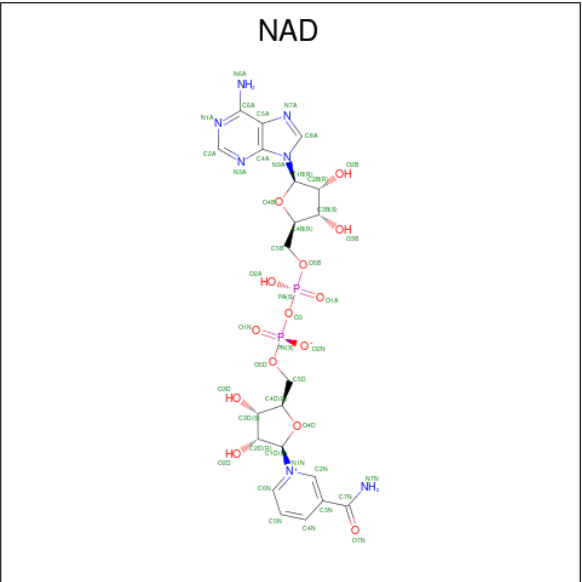
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1210	Total	C	H	N	O	S	0	0	0
			17588	5568	8750	1575	1665	30			
1	B	1209	Total	C	H	N	O	S	0	0	0
			17565	5558	8739	1576	1662	30			

There are 6 discrepancies between the modelled and reference sequences:

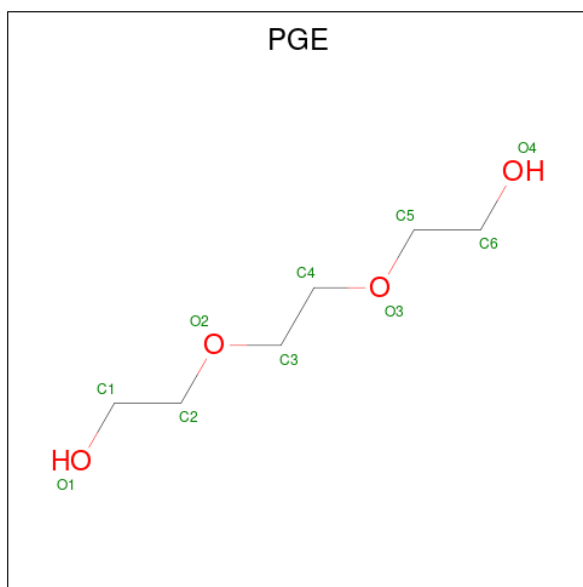
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
A	844	SER	CYS	engineered mutation	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3
B	844	SER	CYS	engineered mutation	UNP F7X6I3

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



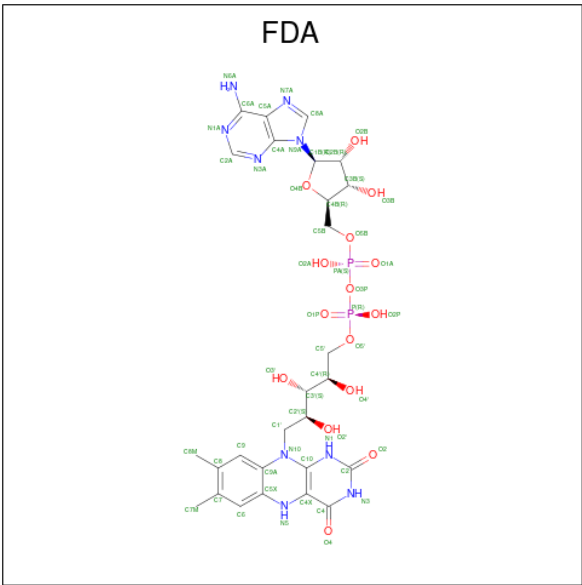
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



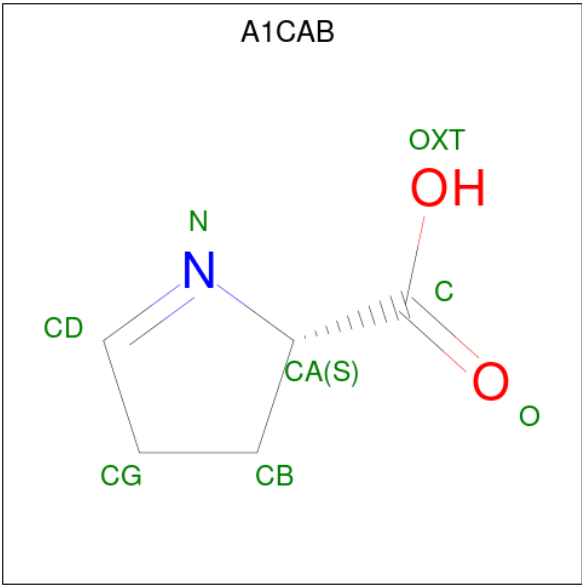
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



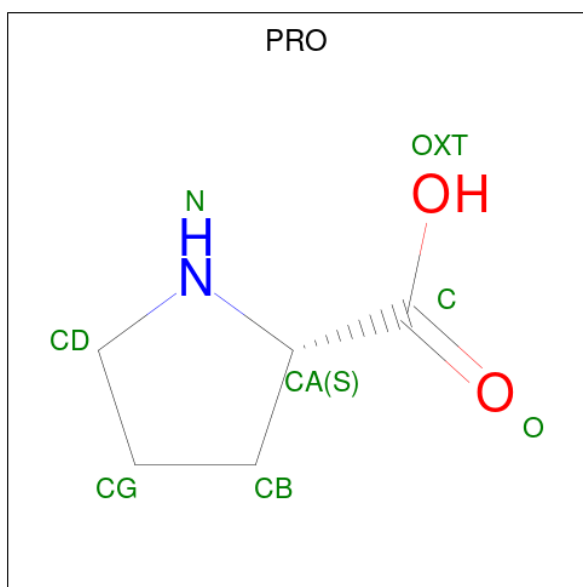
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			86	27	33	9	15		

- Molecule 5 is (2S)-3,4-dihydro-2H-pyrrole-2-carboxylic acid (CCD ID: A1CAB) (formula: C₅H₇NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			15	5	7	1	2		

- Molecule 6 is PROLINE (CCD ID: PRO) (formula: C₅H₉NO₂) (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	9	1	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

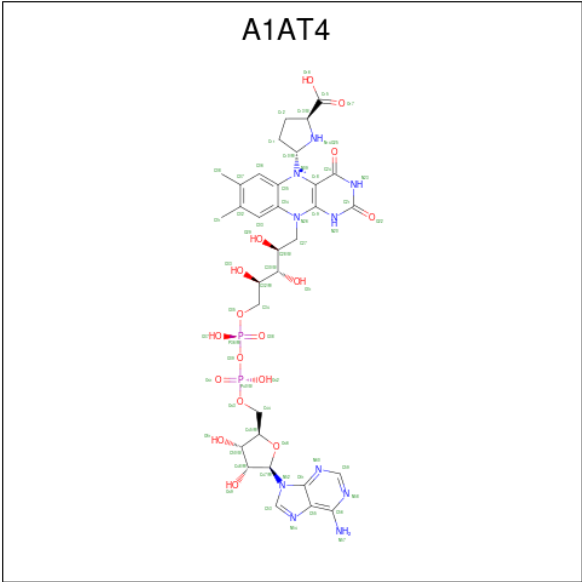
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is (2 {S},5 {R})-5-[10-[(2 {S},3 {S},4 {R})-5-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-2,3,4-tris(oxidanyl)pentyl]-7,8-dimethyl-2,4-bis(oxidanylidene)benzo[g]pteridin-5-yl]pyrrolidine-2-carboxylic acid (CCD ID: A1AT4) (formula: C₃₂H₄₂N₁₀O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	0	0
			100	32	39	10	17	2		

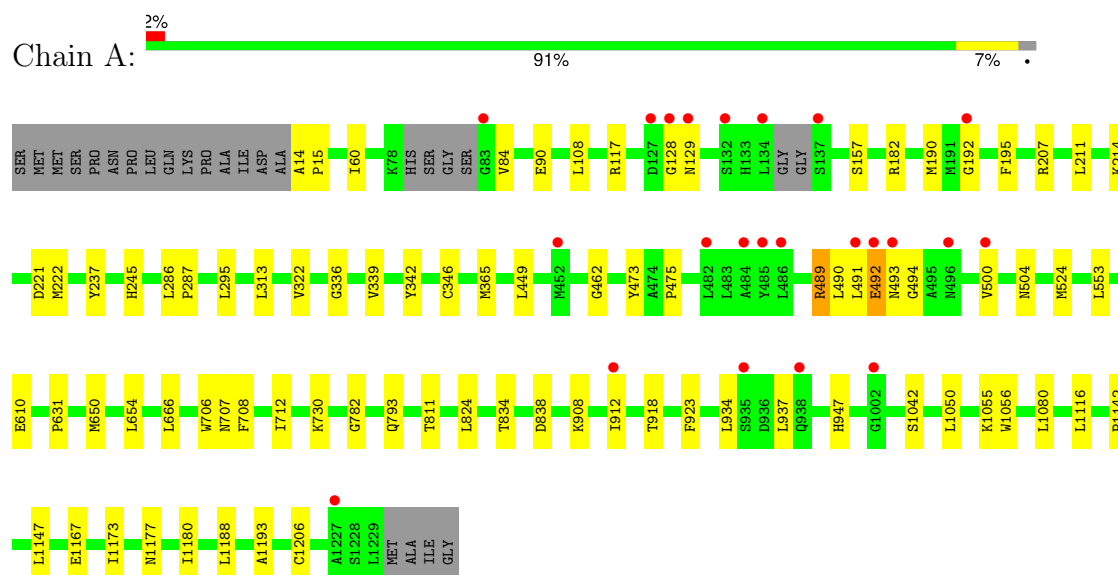
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	621	Total	O	0	0
			621	621		
10	B	658	Total	O	0	0
			658	658		

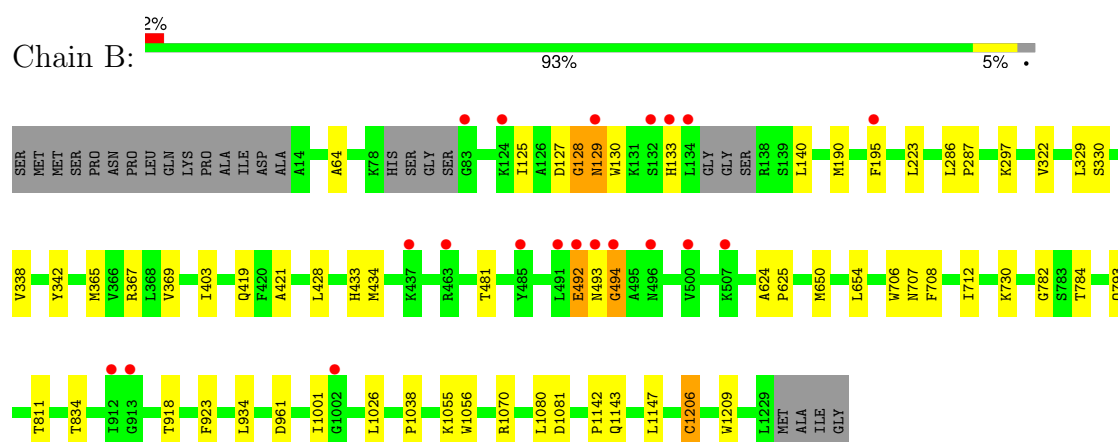
3 Residue-property plots

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

• Molecule 1: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.60Å 102.57Å 127.20Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	67.38 – 1.88 67.38 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.7 (67.38-1.88) 97.0 (67.38-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.21_5207:0000)	Depositor
R, R_{free}	0.170 , 0.206 0.165 , 0.202	Depositor DCC
R_{free} test set	9813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36865	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: SO4, A1CAB, A1AT4, NAD, PGE, FDA, OCS, MG

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	0.45	1/8985 (0.0%)	0.58	1/12248 (0.0%)
1	B	0.47	0/8972	0.59	0/12230
All	All	0.46	1/17957 (0.0%)	0.58	1/24478 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	631	PRO	CA-C	-5.47	1.48	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	GLY	CA-C-O	5.32	125.68	122.22

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	8838	8750	8751	48	0
1	B	8826	8739	8739	34	0
2	A	44	26	26	0	0
2	B	44	26	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	14	14	0	0
3	B	10	14	14	1	0
4	A	53	33	33	2	0
5	A	8	7	0	1	0
6	A	8	9	7	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	15	0	0	0	0
8	B	10	0	0	0	0
9	B	61	39	0	0	0
10	A	621	0	0	4	0
10	B	658	0	0	5	0
All	All	19208	17657	17610	83	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 (83) 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:B:793:GLN:OE1	10:B:2202:HOH:O	2.08	0.70
1:A:793:GLN:OE1	10:A:2201:HOH:O	2.11	0.68
2:B:2101:NAD:O1N	10:B:2201:HOH:O	2.12	0.67
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.76	0.67
1:A:489:ARG:HB2	6:A:2105:PRO:HA	1.83	0.60
1:A:475:PRO:HG3	6:A:2105:PRO:HG2	1.84	0.59
1:B:1143:GLN:O	1:B:1147:LEU:HD13	2.02	0.59
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.39	0.57
1:B:1070:ARG:HD3	10:B:2331:HOH:O	2.05	0.57
1:B:190:MET:HE2	1:B:195:PHE:CZ	2.41	0.56
1:B:784:THR:HG22	1:B:811:THR:HB	1.86	0.56
1:A:60:ILE:HD12	10:A:2742:HOH:O	2.06	0.56
1:B:365:MET:HE3	1:B:419:GLN:OE1	2.05	0.55
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.88	0.55
1:A:449:LEU:HD13	1:A:489:ARG:HD2	1.89	0.54
1:A:489:ARG:NE	1:A:489:ARG:HA	2.22	0.54
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.90	0.52
1:B:492:GLU:O	1:B:494:GLY:N	2.42	0.51
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.46	0.51
1:A:650:MET:O	1:A:654:LEU:HG	2.10	0.51
1:B:428:LEU:C	1:B:428:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:PHE:HB2	1:B:712:ILE:HD12	1.94	0.50
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.92	0.50
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.47	0.50
1:A:937:LEU:HD21	1:A:947:HIS:CD2	2.47	0.49
1:A:286:LEU:HB3	1:A:287:PRO:HD3	1.94	0.48
1:A:708:PHE:HB2	1:A:712:ILE:HD12	1.95	0.48
1:B:782:GLY:O	1:B:811:THR:HA	2.14	0.48
1:A:221:ASP:HB2	1:A:473:TYR:CZ	2.50	0.47
1:A:918:THR:HB	1:A:923:PHE:CD1	2.49	0.47
1:B:650:MET:O	1:B:654:LEU:HG	2.14	0.47
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	1.97	0.47
10:A:2237:HOH:O	1:B:1055:LYS:HE3	2.15	0.46
1:B:403:ILE:HG23	1:B:434:MET:HE1	1.98	0.46
1:B:128:GLY:O	1:B:130:TRP:N	2.44	0.46
1:A:108:LEU:O	1:A:117:ARG:HD3	2.14	0.46
1:B:330:SER:HB2	10:B:2303:HOH:O	2.15	0.46
1:A:128:GLY:O	1:A:129:ASN:C	2.58	0.46
1:A:90:GLU:OE1	1:A:182:ARG:NH2	2.31	0.46
1:A:489:ARG:HA	1:A:489:ARG:CZ	2.45	0.46
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.51	0.45
1:A:211:LEU:HD23	1:A:214:LYS:HD3	1.98	0.45
1:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.44	0.45
1:A:192:GLY:O	1:A:207:ARG:NH1	2.49	0.45
1:A:782:GLY:O	1:A:811:THR:HA	2.16	0.45
1:A:490:LEU:O	1:A:491:LEU:C	2.59	0.45
1:A:500:VAL:O	1:A:504:ASN:ND2	2.51	0.44
1:A:339:VAL:HG12	1:A:346:CYS:SG	2.57	0.44
1:B:127:ASP:O	1:B:129:ASN:N	2.51	0.44
1:A:222:MET:HG2	10:A:2253:HOH:O	2.18	0.43
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.43	0.43
1:A:336:GLY:HA2	1:A:365:MET:O	2.19	0.43
1:A:834:THR:O	1:A:838:ASP:HB2	2.19	0.43
1:A:1147:LEU:HD22	1:B:1147:LEU:HG	1.99	0.43
1:B:624:ALA:HB3	1:B:625:PRO:HD3	2.01	0.43
1:B:369:VAL:HG12	1:B:421:ALA:HB3	2.01	0.42
1:B:338:VAL:HG22	1:B:367:ARG:HB3	2.00	0.42
1:A:237:TYR:CD1	1:A:237:TYR:C	2.97	0.42
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.54	0.42
1:B:286:LEU:HB3	1:B:287:PRO:HD3	2.01	0.42
1:A:473:TYR:HB2	4:A:2103:FDA:HM72	2.02	0.42
1:B:125:ILE:O	1:B:128:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:C	1:A:313:LEU:HD23	2.45	0.42
1:A:492:GLU:O	1:A:494:GLY:N	2.53	0.42
4:A:2103:FDA:N5	5:A:2104:A1CAB:CD	2.83	0.42
1:A:1167:GLU:HA	1:A:1193:ALA:O	2.20	0.41
1:A:489:ARG:NE	1:A:489:ARG:CA	2.82	0.41
1:A:553:LEU:HD12	1:A:666:LEU:HG	2.02	0.41
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.55	0.41
1:B:1206:OCS:HB2	1:B:1209:TRP:CD1	2.56	0.41
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.54	0.41
1:A:449:LEU:HD13	1:A:489:ARG:CD	2.49	0.41
1:A:937:LEU:HD21	1:A:947:HIS:NE2	2.35	0.41
1:A:14:ALA:HA	1:A:15:PRO:HD3	1.94	0.41
1:B:223:LEU:HB3	1:B:481:THR:HG22	2.03	0.41
1:B:834:THR:HG22	1:B:1001:ILE:HD11	2.02	0.41
1:B:918:THR:HB	1:B:923:PHE:CD1	2.56	0.41
1:A:489:ARG:CB	6:A:2105:PRO:HA	2.48	0.41
1:A:1173:ILE:O	1:A:1177:ASN:HB2	2.20	0.41
3:B:2102:PGE:C1	10:B:2222:HOH:O	2.70	0.40
1:A:908:LYS:NZ	1:A:908:LYS:HB3	2.36	0.40
1:A:1042:SER:O	1:A:1080:LEU:HD13	2.21	0.40
1:B:1080:LEU:HD12	1:B:1081:ASP:H	1.86	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	1203/1235 (97%)	1173 (98%)	28 (2%)	2 (0%)	44	34
1	B	1202/1235 (97%)	1171 (97%)	25 (2%)	6 (0%)	25	13
All	All	2405/2470 (97%)	2344 (98%)	53 (2%)	8 (0%)	37	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	GLU
1	B	492	GLU
1	A	493	ASN
1	B	493	ASN
1	B	128	GLY
1	B	129	ASN
1	B	133	HIS
1	B	494	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	868/950 (91%)	857 (99%)	11 (1%)	65	55
1	B	866/950 (91%)	862 (100%)	4 (0%)	86	84
All	All	1734/1900 (91%)	1719 (99%)	15 (1%)	75	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	157	SER
1	A	342	TYR
1	A	489	ARG
1	A	524	MET
1	A	610	GLU
1	A	730	LYS
1	A	824	LEU
1	A	912	ILE
1	A	934	LEU
1	A	1116	LEU
1	B	140	LEU
1	B	342	TYR
1	B	730	LYS
1	B	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	504	ASN
1	B	504	ASN
1	B	667	ASN
1	B	685	GLN
1	B	791	GLN
1	B	872	HIS
1	B	1115	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	B	1206	1	6,8,9	1.47	1 (16%)	7,11,13	1.60	2 (28%)
1	OCS	A	1206	1	6,8,9	1.41	1 (16%)	7,11,13	1.63	2 (28%)

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
1	OCS	B	1206	1	-	1/4/7/9	-
1	OCS	A	1206	1	-	1/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1206	OCS	CB-CA	-2.74	1.51	1.53
1	A	1206	OCS	CB-CA	-2.63	1.51	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1206	OCS	OD3-SG-CB	-3.06	102.19	106.76
1	A	1206	OCS	OD2-SG-OD3	2.59	117.87	111.40
1	A	1206	OCS	OD3-SG-CB	-2.33	103.27	106.76
1	B	1206	OCS	OD2-SG-OD3	2.11	116.67	111.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1206	OCS	N-CA-CB-SG
1	B	1206	OCS	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1206	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
9	A1AT4	B	2103	-	62,67,67	2.27	10 (16%)	72,103,103	1.37	10 (13%)
3	PGE	A	2102	-	9,9,9	0.33	0	8,8,8	0.47	0
2	NAD	A	2101	7	42,48,48	2.18	12 (28%)	50,73,73	1.54	7 (14%)
8	SO4	A	2108	-	4,4,4	0.71	0	6,6,6	0.26	0
3	PGE	B	2102	-	9,9,9	0.38	0	8,8,8	0.65	0
2	NAD	B	2101	7	42,48,48	2.51	13 (30%)	50,73,73	1.71	8 (16%)
8	SO4	B	2106	-	4,4,4	0.74	0	6,6,6	0.12	0
5	A1CAB	A	2104	-	7,8,8	4.84	2 (28%)	6,10,10	1.26	1 (16%)
8	SO4	A	2107	-	4,4,4	0.51	0	6,6,6	0.31	0
8	SO4	A	2109	-	4,4,4	0.75	0	6,6,6	0.32	0
8	SO4	B	2105	-	4,4,4	0.46	0	6,6,6	0.15	0
4	FDA	A	2103	-	53,58,58	2.10	14 (26%)	64,89,89	1.20	10 (15%)
6	PRO	A	2105	-	8,8,8	1.73	1 (12%)	10,10,10	1.48	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
9	A1AT4	B	2103	-	-	6/34/67/67	0/6/7/7
3	PGE	A	2102	-	-	4/7/7/7	-
2	NAD	A	2101	7	-	1/26/62/62	0/5/5/5
3	PGE	B	2102	-	-	3/7/7/7	-
2	NAD	B	2101	7	-	2/26/62/62	0/5/5/5
5	A1CAB	A	2104	-	-	2/4/11/11	0/1/1/1
4	FDA	A	2103	-	-	4/30/50/50	0/6/6/6
6	PRO	A	2105	-	-	3/4/11/11	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2104	A1CAB	CD-N	12.50	1.34	1.26
9	B	2103	A1AT4	C10-N09	11.01	1.67	1.48
4	A	2103	FDA	P-O3P	8.68	1.68	1.59
2	B	2101	NAD	C2N-N1N	8.33	1.44	1.35
9	B	2103	A1AT4	P36-O39	8.11	1.68	1.59
2	A	2101	NAD	C2N-N1N	7.15	1.42	1.35
2	A	2101	NAD	PA-O3	-6.61	1.52	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2101	NAD	PN-O3	6.21	1.66	1.59
2	B	2101	NAD	C7N-N7N	5.84	1.43	1.33
2	B	2101	NAD	PA-O3	-5.60	1.53	1.59
9	B	2103	A1AT4	C18-N09	5.26	1.46	1.37
2	A	2101	NAD	C7N-N7N	4.81	1.41	1.33
4	A	2103	FDA	C4X-N5	4.26	1.44	1.35
9	B	2103	A1AT4	C05-N09	4.20	1.48	1.42
6	A	2105	PRO	CA-C	4.16	1.63	1.52
4	A	2103	FDA	C5X-N5	3.96	1.46	1.39
4	A	2103	FDA	C4-N3	3.66	1.45	1.38
4	A	2103	FDA	C5'-C4'	3.65	1.56	1.51
9	B	2103	A1AT4	O46-C47	3.56	1.45	1.40
4	A	2103	FDA	O4B-C1B	3.45	1.45	1.40
9	B	2103	A1AT4	C34-C32	3.12	1.56	1.51
4	A	2103	FDA	C2-N1	2.93	1.42	1.37
2	B	2101	NAD	C6N-N1N	2.83	1.41	1.35
2	A	2101	NAD	C6N-N1N	2.82	1.41	1.35
2	B	2101	NAD	C6A-N6A	2.74	1.43	1.34
4	A	2103	FDA	P-O5'	2.73	1.70	1.59
2	B	2101	NAD	C2A-N3A	2.58	1.36	1.32
2	A	2101	NAD	PA-O5B	-2.56	1.49	1.59
9	B	2103	A1AT4	C59-N58	2.56	1.38	1.33
2	B	2101	NAD	PA-O2A	-2.50	1.43	1.55
4	A	2103	FDA	C2A-N3A	2.49	1.35	1.32
4	A	2103	FDA	C9-C8	2.43	1.42	1.39
2	B	2101	NAD	C1B-N9A	-2.38	1.44	1.49
2	A	2101	NAD	C4N-C3N	2.38	1.43	1.39
2	B	2101	NAD	O2B-C2B	-2.36	1.37	1.43
4	A	2103	FDA	C9A-N10	2.35	1.45	1.41
2	A	2101	NAD	C5N-C4N	2.30	1.42	1.38
2	A	2101	NAD	C6A-N6A	2.29	1.42	1.34
2	A	2101	NAD	C2A-N3A	2.26	1.35	1.32
9	B	2103	A1AT4	P36-O35	2.21	1.68	1.59
2	B	2101	NAD	PA-O5B	-2.18	1.50	1.59
2	A	2101	NAD	C1B-N9A	-2.18	1.44	1.49
2	B	2101	NAD	C5N-C4N	2.14	1.42	1.38
4	A	2103	FDA	C2A-N1A	2.14	1.37	1.33
4	A	2103	FDA	PA-O1A	2.14	1.58	1.50
9	B	2103	A1AT4	C59-N60	2.13	1.35	1.32
5	A	2104	A1CAB	CA-C	2.06	1.54	1.52
4	A	2103	FDA	C2'-C3'	2.05	1.57	1.53
2	A	2101	NAD	O4B-C1B	2.03	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2101	NAD	O2B-C2B	-2.03	1.37	1.43
2	B	2101	NAD	O4B-C1B	2.03	1.43	1.40
9	B	2103	A1AT4	P40-O41	2.02	1.57	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2101	NAD	N3A-C2A-N1A	-7.22	118.87	128.67
2	A	2101	NAD	N3A-C2A-N1A	-6.66	119.63	128.67
9	B	2103	A1AT4	C05-N09-C18	-4.06	110.48	120.01
6	A	2105	PRO	OXT-C-O	3.55	132.13	124.08
2	B	2101	NAD	C6N-N1N-C2N	-3.49	118.91	121.88
4	A	2103	FDA	C5X-N5-C4X	-3.05	114.04	121.08
2	B	2101	NAD	C4B-O4B-C1B	-3.00	107.18	109.92
2	A	2101	NAD	C4B-O4B-C1B	-2.98	107.20	109.92
2	B	2101	NAD	C2N-C3N-C4N	2.97	121.71	118.26
9	B	2103	A1AT4	O43-P40-O41	-2.91	97.40	108.94
9	B	2103	A1AT4	C47-N52-C61	-2.90	121.54	126.64
9	B	2103	A1AT4	C18-C24-N23	2.85	115.95	110.94
9	B	2103	A1AT4	C12-C13-C15	-2.83	105.42	112.72
2	A	2101	NAD	O5B-PA-O1A	2.80	120.03	108.94
6	A	2105	PRO	O-C-CA	-2.79	113.25	122.26
4	A	2103	FDA	C1'-C2'-C3'	2.73	117.05	109.66
9	B	2103	A1AT4	O17-C15-C13	-2.57	113.96	122.26
2	A	2101	NAD	C1B-N9A-C4A	-2.48	122.28	126.64
2	B	2101	NAD	O2N-PN-O3	2.46	113.92	107.27
4	A	2103	FDA	O3P-P-O1P	-2.44	103.37	110.70
2	A	2101	NAD	C6N-N1N-C2N	-2.42	119.82	121.88
9	B	2103	A1AT4	O16-C15-C13	2.34	121.44	113.51
4	A	2103	FDA	C5A-C6A-N6A	2.34	123.87	120.31
2	A	2101	NAD	C4A-C5A-N7A	-2.31	106.89	109.34
5	A	2104	A1CAB	CB-CG-CD	2.29	105.49	102.73
4	A	2103	FDA	O2P-P-O1P	2.27	122.99	112.44
9	B	2103	A1AT4	C24-N23-C21	-2.25	123.27	126.37
2	B	2101	NAD	O2A-PA-O3	-2.23	101.24	107.27
2	B	2101	NAD	C5N-C4N-C3N	-2.22	118.18	120.36
4	A	2103	FDA	O5B-PA-O1A	-2.20	100.20	108.94
2	B	2101	NAD	O5B-C5B-C4B	2.20	116.49	108.99
9	B	2103	A1AT4	C15-C13-N14	2.14	115.31	106.93
4	A	2103	FDA	C1B-N9A-C4A	-2.14	122.88	126.64
4	A	2103	FDA	O3'-C3'-C2'	-2.13	104.09	108.93
4	A	2103	FDA	C9A-C5X-N5	2.11	121.95	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2103	A1AT4	O25-C24-C18	-2.06	122.56	127.62
2	A	2101	NAD	O5B-C5B-C4B	2.02	115.87	108.99
4	A	2103	FDA	O5B-C5B-C4B	-2.01	102.17	108.99

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2101	NAD	C5B-O5B-PA-O1A
5	A	2104	A1CAB	O-C-CA-N
9	B	2103	A1AT4	O31-C30-C32-O33
9	B	2103	A1AT4	O31-C30-C32-C34
9	B	2103	A1AT4	C28-C30-C32-O33
3	A	2102	PGE	O2-C3-C4-O3
4	A	2103	FDA	P-O3P-PA-O5B
9	B	2103	A1AT4	P36-O39-P40-O43
3	B	2102	PGE	O3-C5-C6-O4
3	B	2102	PGE	C1-C2-O2-C3
2	B	2101	NAD	C4D-C5D-O5D-PN
3	A	2102	PGE	O3-C5-C6-O4
2	A	2101	NAD	C4D-C5D-O5D-PN
3	A	2102	PGE	C4-C3-O2-C2
6	A	2105	PRO	O-C-CA-CB
3	A	2102	PGE	O1-C1-C2-O2
3	B	2102	PGE	O2-C3-C4-O3
9	B	2103	A1AT4	C32-C34-O35-P36
4	A	2103	FDA	O3'-C3'-C4'-C5'
5	A	2104	A1CAB	OXT-C-CA-N
6	A	2105	PRO	O-C-CA-N
4	A	2103	FDA	O3'-C3'-C4'-O4'
6	A	2105	PRO	OXT-C-CA-CB
4	A	2103	FDA	C4'-C5'-O5'-P
9	B	2103	A1AT4	C28-C30-C32-C34

There are no ring outliers.

5 monomers are involved in 7 short contacts:

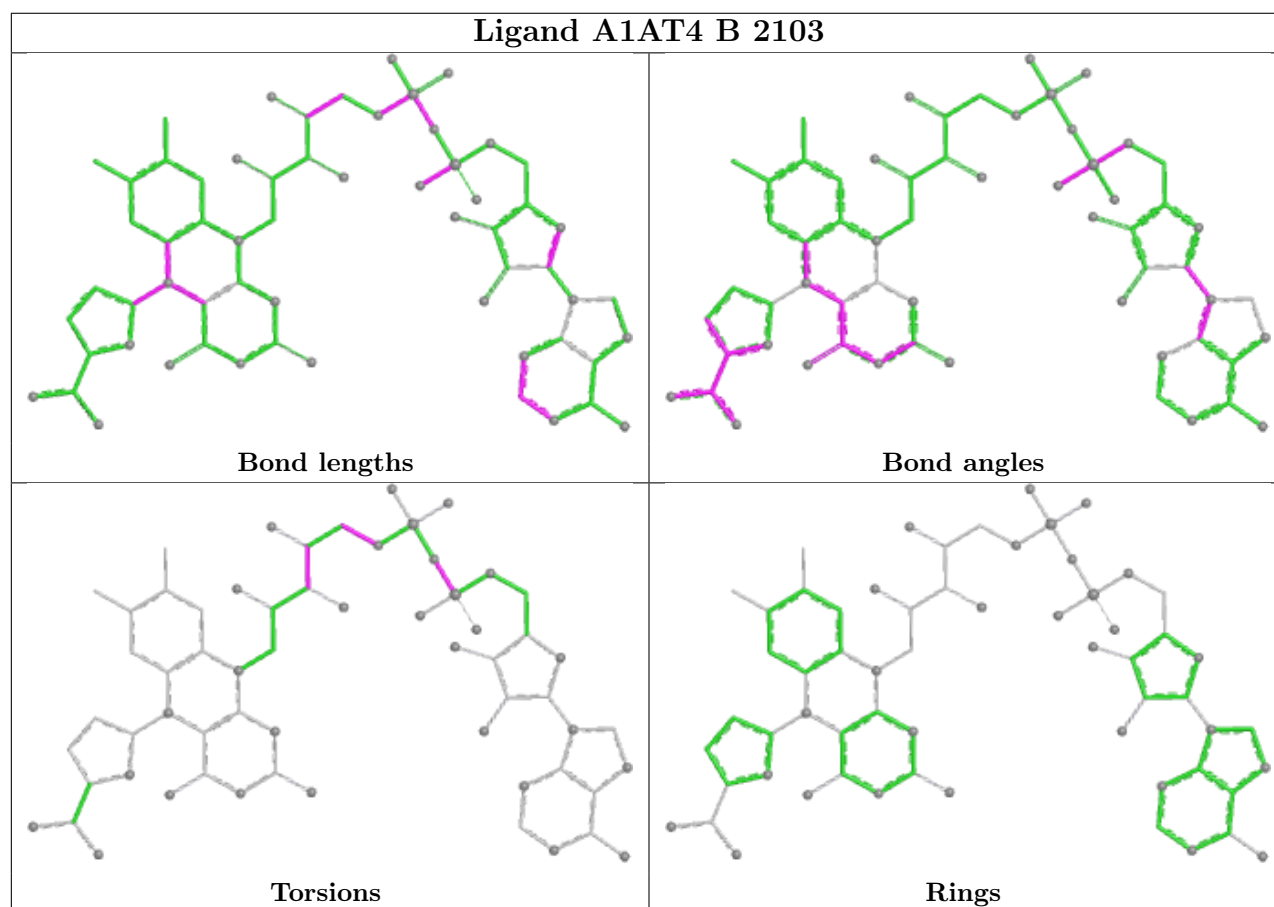
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2102	PGE	1	0
2	B	2101	NAD	1	0
5	A	2104	A1CAB	1	0

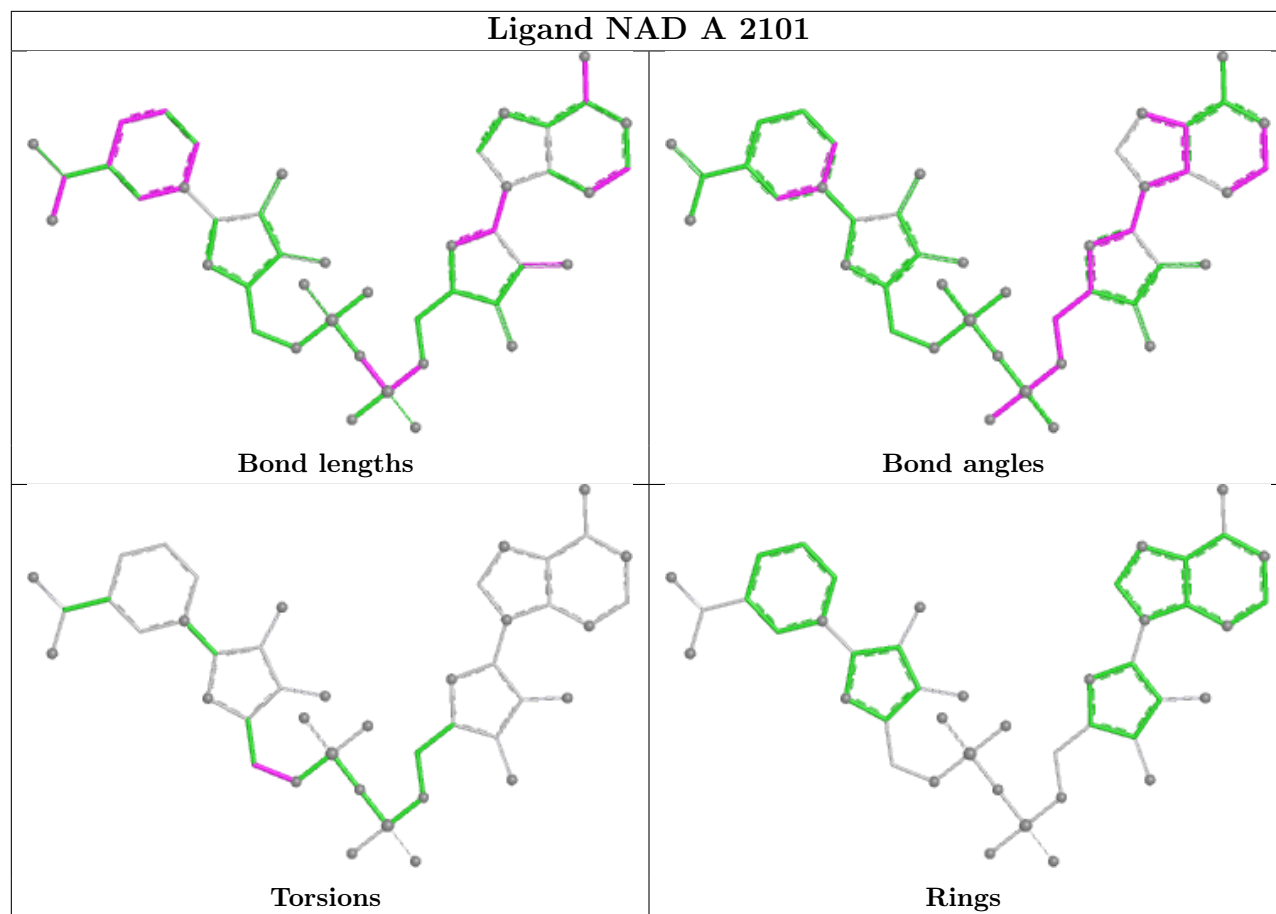
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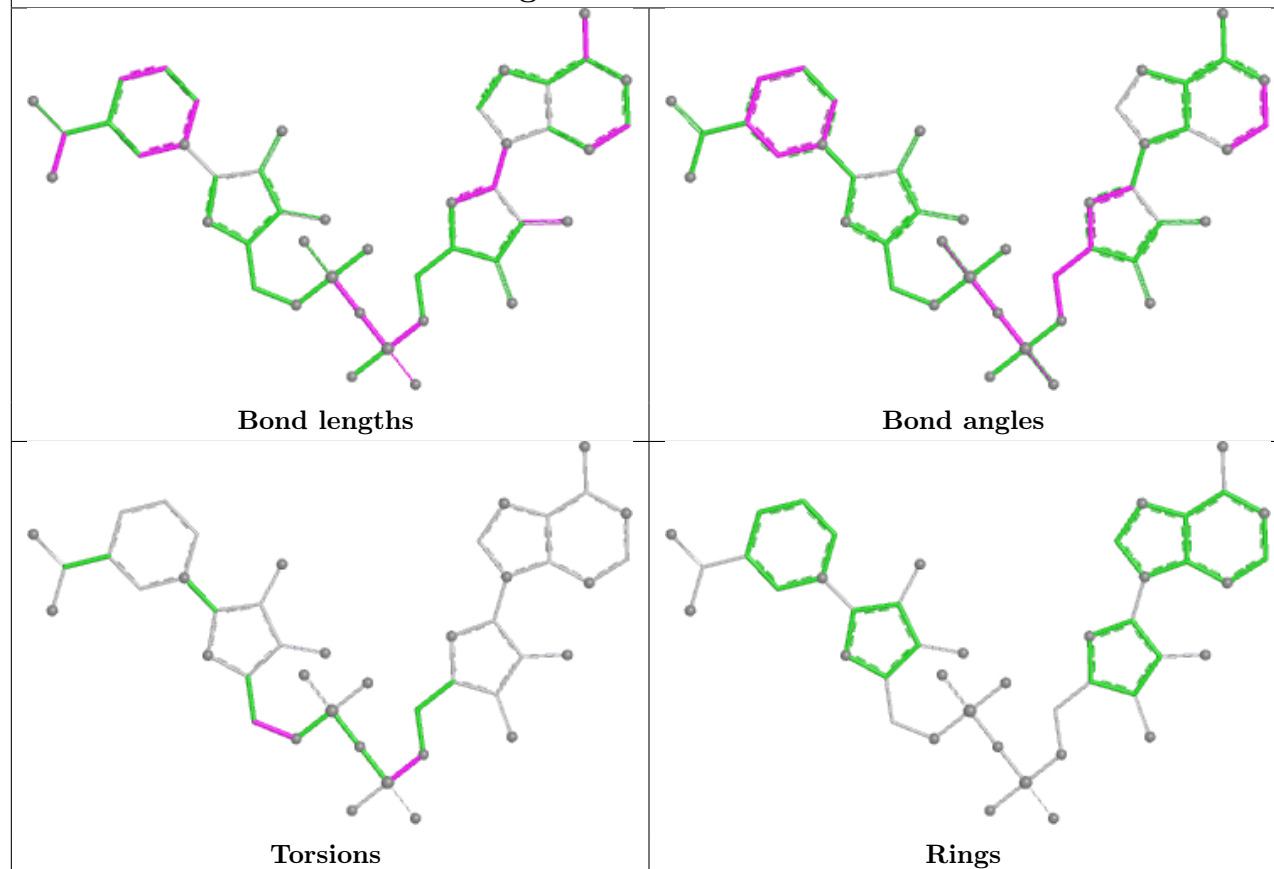
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2103	FDA	2	0
6	A	2105	PRO	3	0

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.

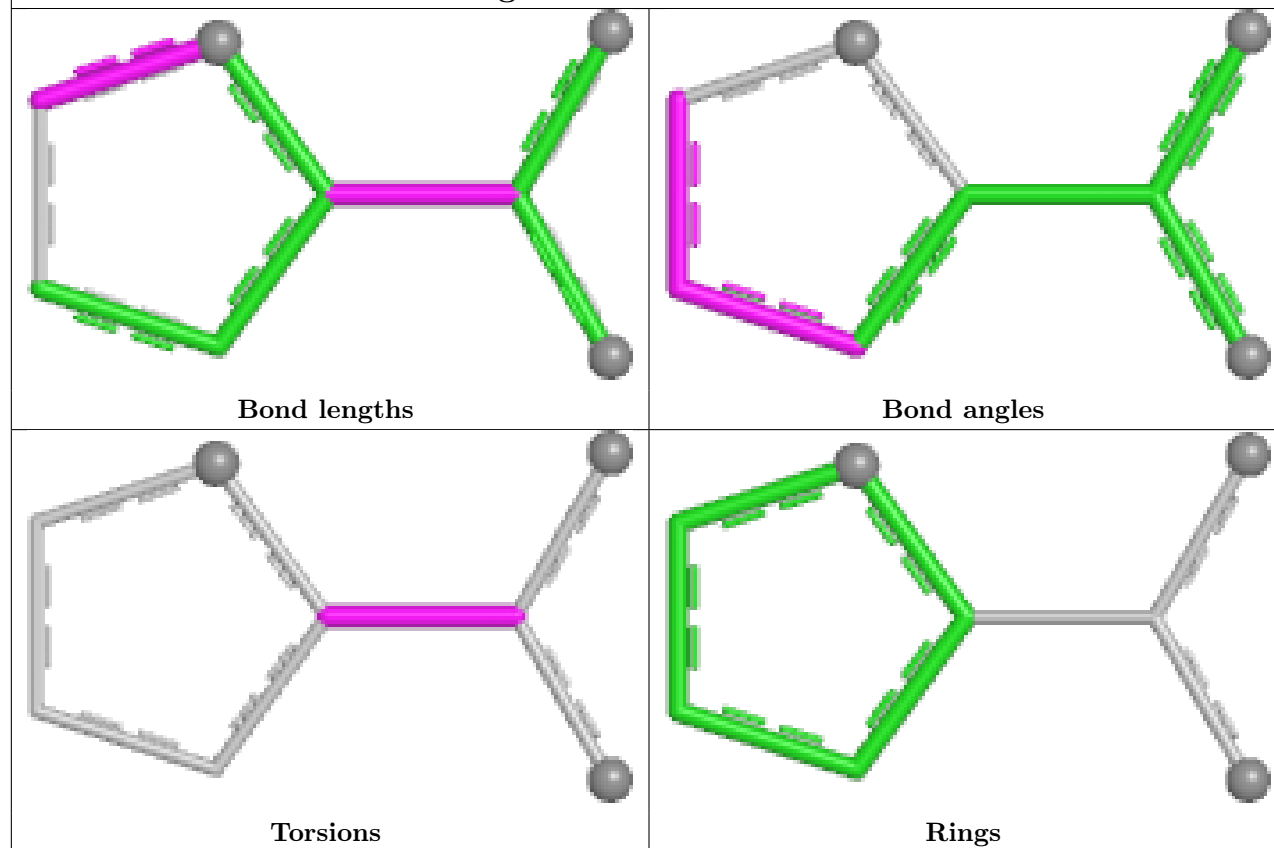


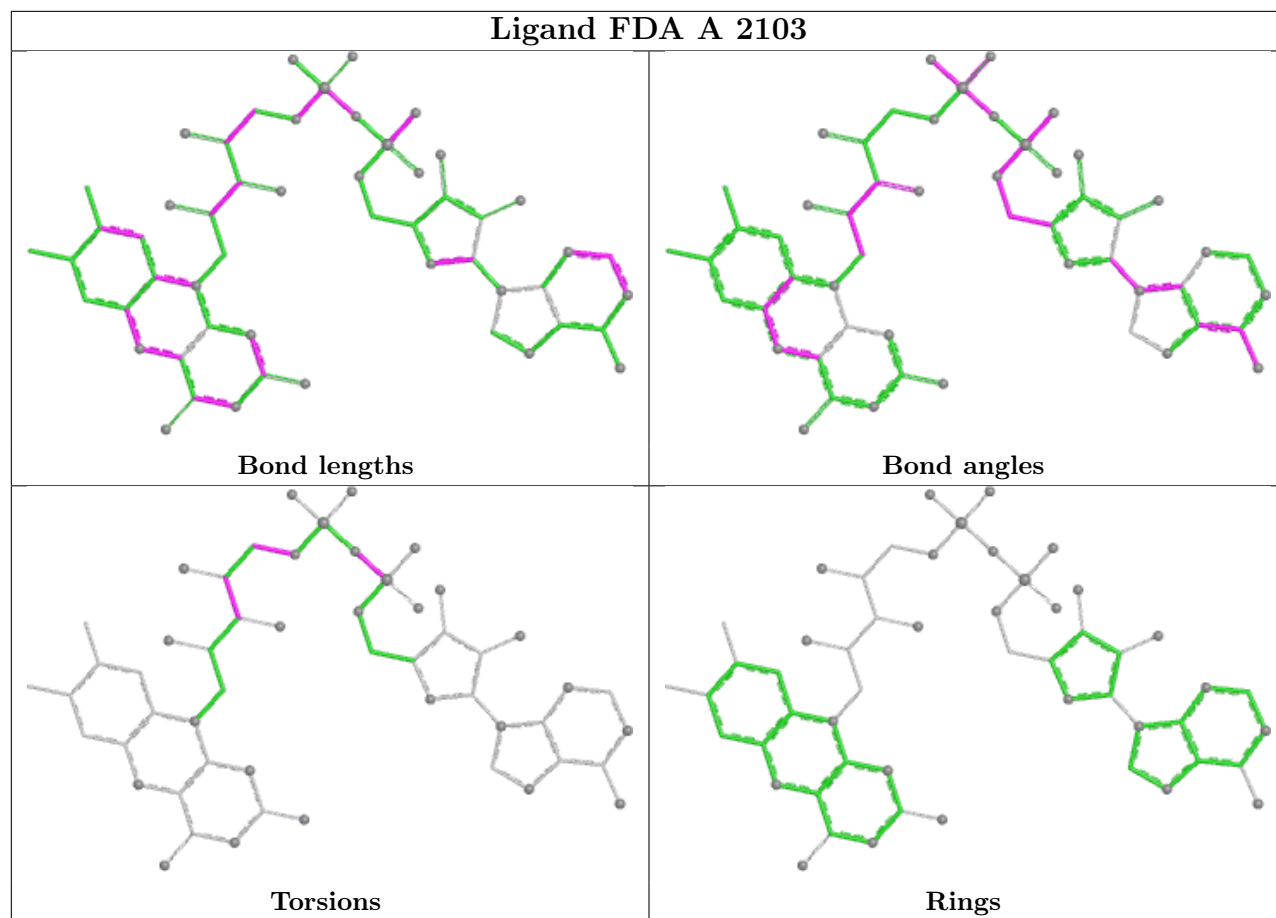


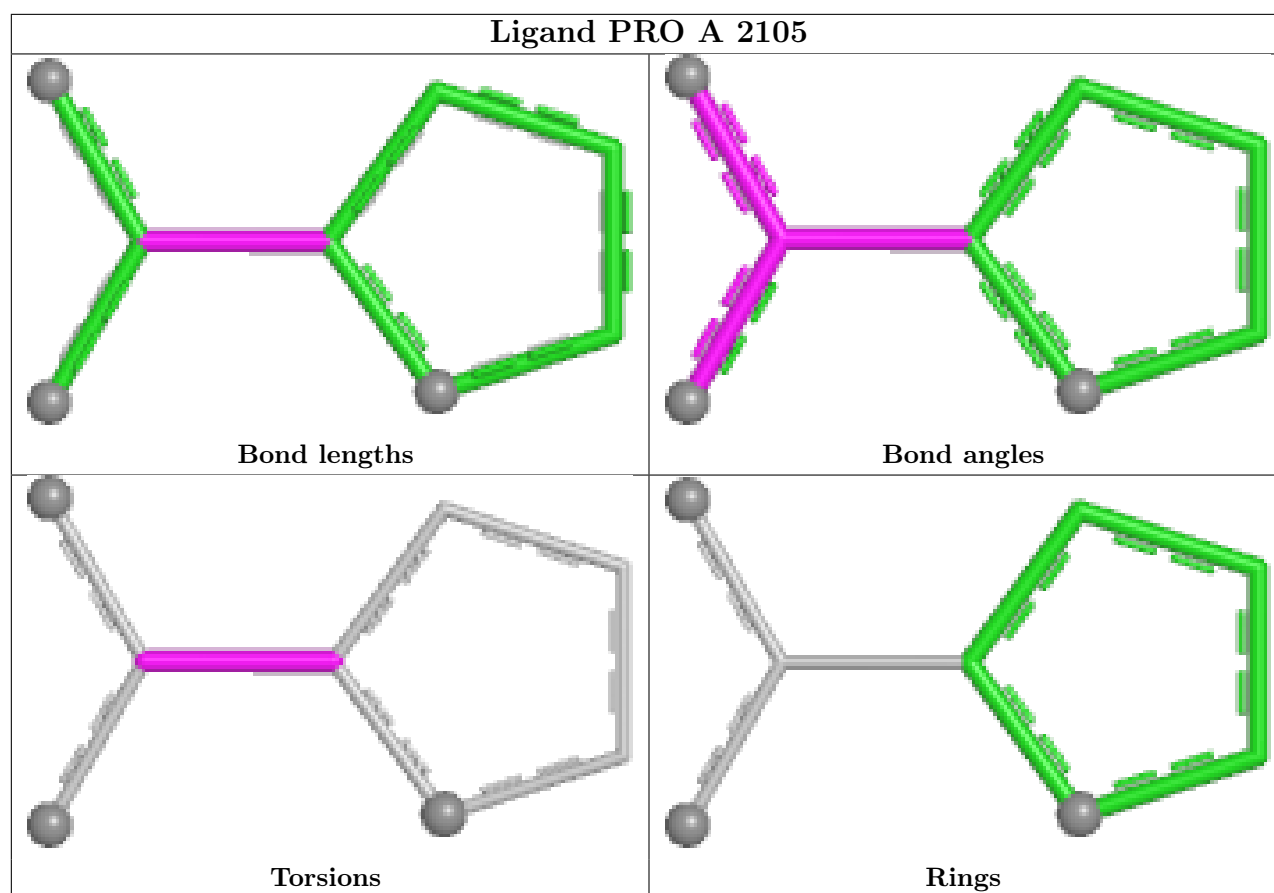
Ligand NAD B 2101



Ligand A1CAB A 2104







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	1209/1235 (97%)	-0.35	23 (1%) 66 71	21, 34, 58, 92	0
1	B	1208/1235 (97%)	-0.37	20 (1%) 69 74	20, 32, 57, 86	0
All	All	2417/2470 (97%)	-0.36	43 (1%) 67 72	20, 33, 57, 92	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	ASN	5.0
1	A	134	LEU	4.5
1	A	129	ASN	4.1
1	A	491	LEU	4.0
1	B	491	LEU	3.9
1	A	492	GLU	3.6
1	B	496	ASN	3.5
1	B	912	ILE	3.5
1	A	485	TYR	3.4
1	B	493	ASN	3.4
1	B	129	ASN	3.4
1	B	913	GLY	3.3
1	A	1227	ALA	3.0
1	B	134	LEU	2.9
1	A	127	ASP	2.9
1	A	132	SER	2.9
1	A	500	VAL	2.7
1	B	83	GLY	2.7
1	A	137	SER	2.7
1	A	83	GLY	2.6
1	B	1002	GLY	2.6
1	A	128	GLY	2.6
1	B	492	GLU	2.6
1	A	486	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1002	GLY	2.5
1	B	485	TYR	2.5
1	B	500	VAL	2.5
1	A	484	ALA	2.4
1	B	437	LYS	2.4
1	A	496	ASN	2.3
1	A	482	LEU	2.3
1	B	133	HIS	2.3
1	A	938	GLN	2.3
1	A	935	SER	2.2
1	B	494	GLY	2.2
1	B	124	LYS	2.2
1	B	463	ARG	2.2
1	B	132	SER	2.1
1	B	507	LYS	2.1
1	A	192	GLY	2.1
1	A	912	ILE	2.1
1	A	452	MET	2.1
1	B	195	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	A	1206	9/10	0.95	0.08	25,34,42,47	0
1	OCS	B	1206	9/10	0.96	0.06	23,32,43,47	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

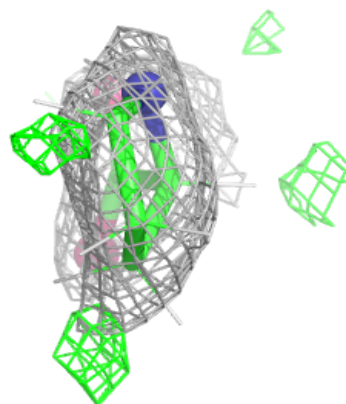
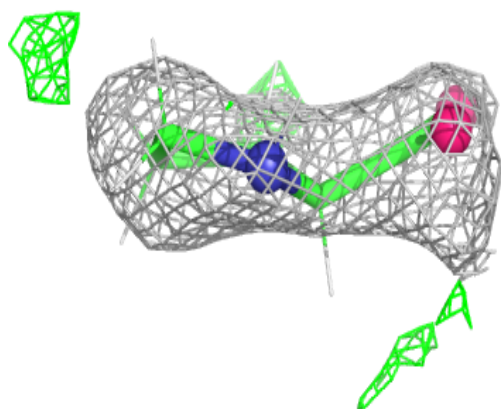
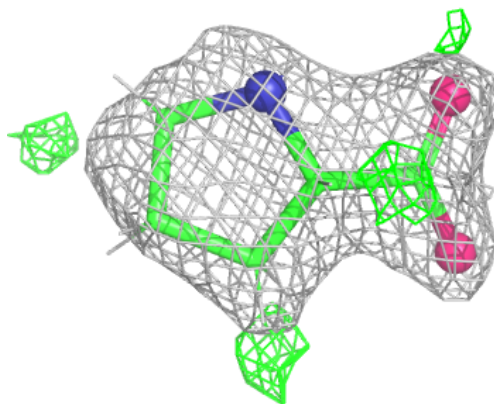
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SO4	B	2106	5/5	0.80	0.09	68,72,76,77	0
6	PRO	A	2105	8/8	0.83	0.15	51,58,66,66	17
3	PGE	A	2102	10/10	0.84	0.12	37,48,58,69	0
5	A1CAB	A	2104	8/8	0.86	0.14	37,44,50,51	15
3	PGE	B	2102	10/10	0.89	0.10	38,50,62,65	0
8	SO4	A	2108	5/5	0.90	0.08	51,52,55,61	0
8	SO4	A	2109	5/5	0.93	0.09	37,42,52,59	5
4	FDA	A	2103	53/53	0.96	0.06	22,35,42,50	0
2	NAD	B	2101	44/44	0.96	0.07	21,29,38,41	0
9	A1AT4	B	2103	61/61	0.96	0.07	24,32,42,47	0
2	NAD	A	2101	44/44	0.97	0.06	25,32,38,42	0
7	MG	A	2106	1/1	0.97	0.04	42,42,42,42	0
7	MG	B	2104	1/1	0.98	0.04	31,31,31,31	0
8	SO4	A	2107	5/5	0.99	0.05	27,28,29,30	0
8	SO4	B	2105	5/5	0.99	0.04	22,26,29,34	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.

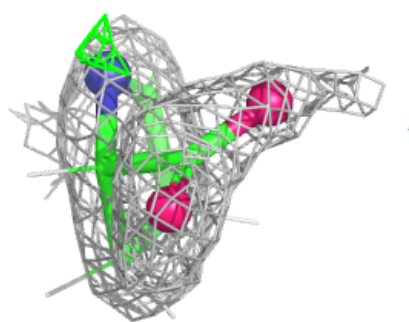
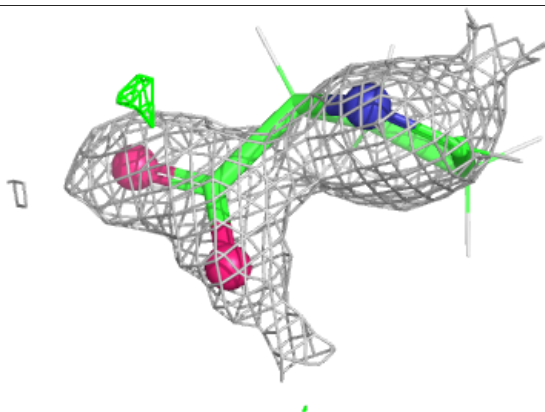
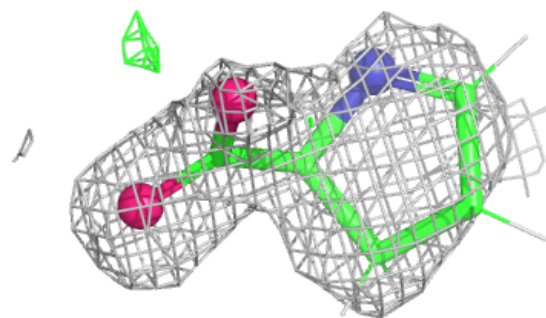
Electron density around PRO A 2105:

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

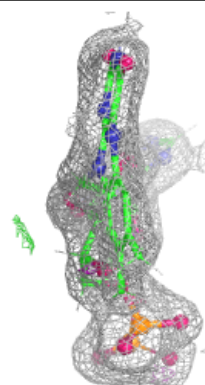
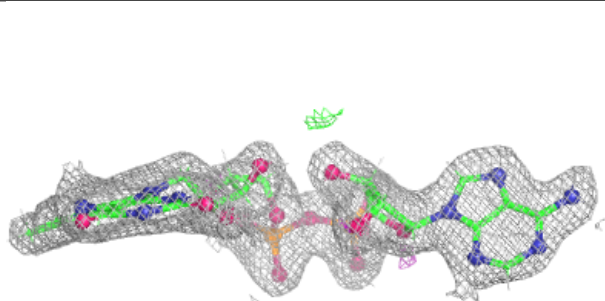
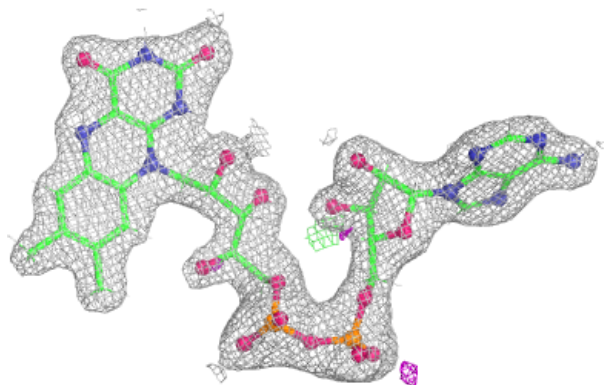


Electron density around A1CAB A 2104:

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

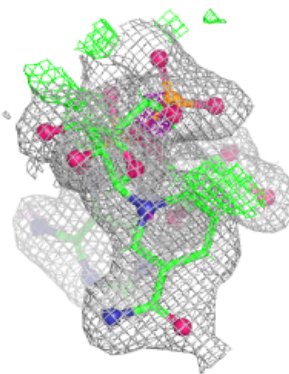
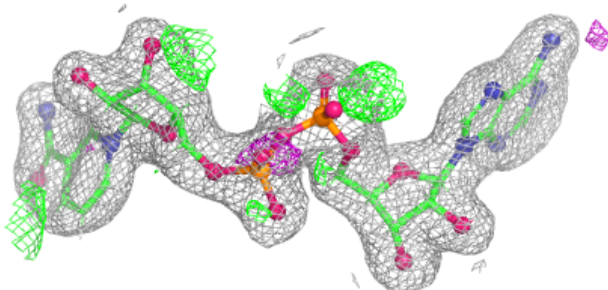
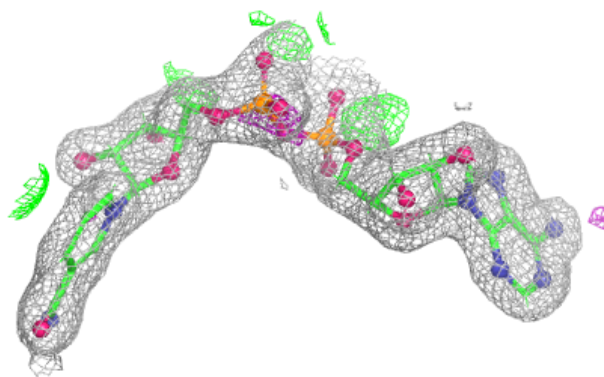
**Electron density around FDA A 2103:**

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

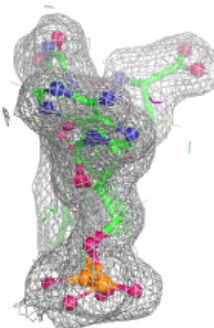
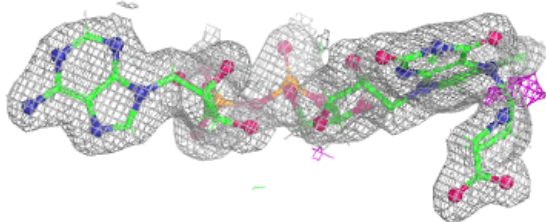
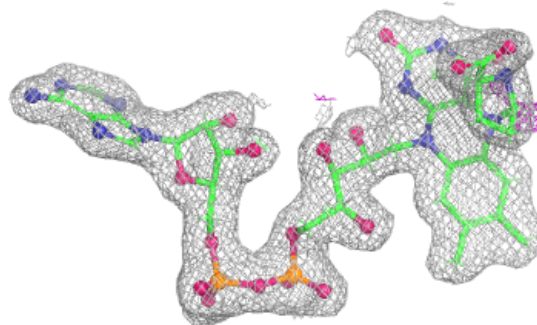


Electron density around NAD B 2101:

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

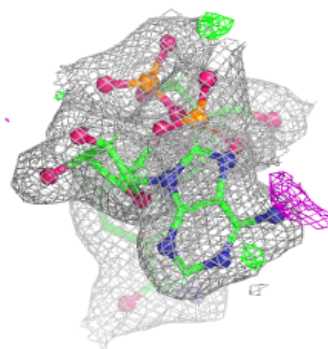
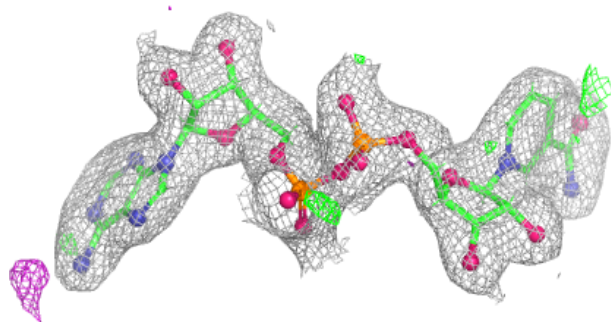
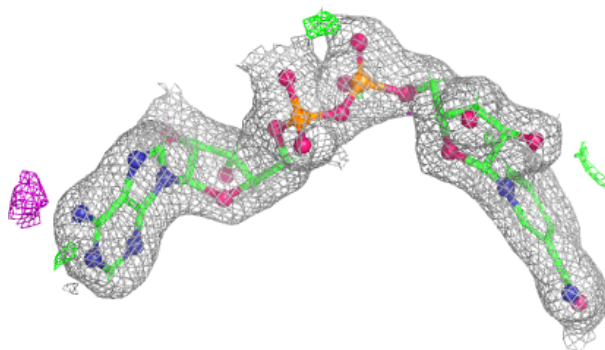
**Electron density around A1AT4 B 2103:**

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



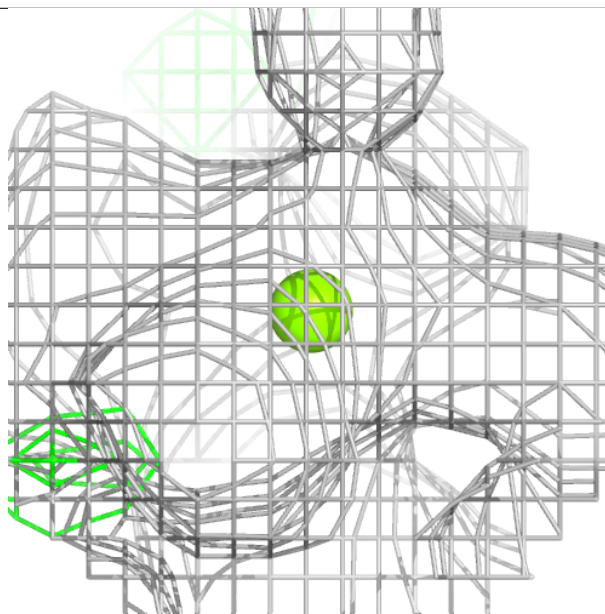
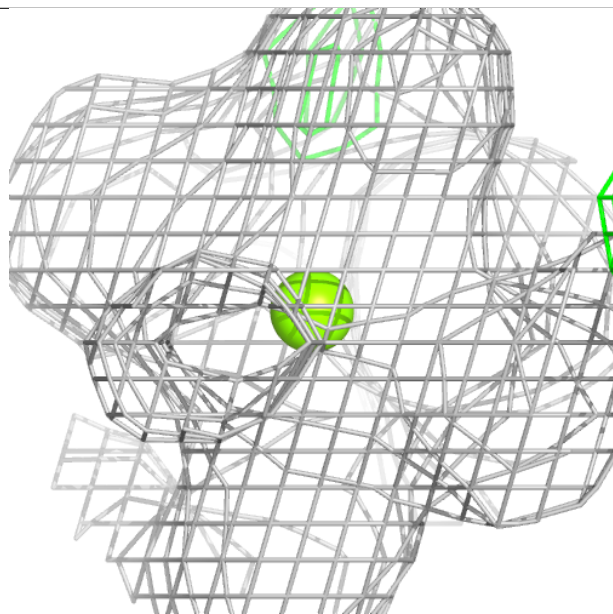
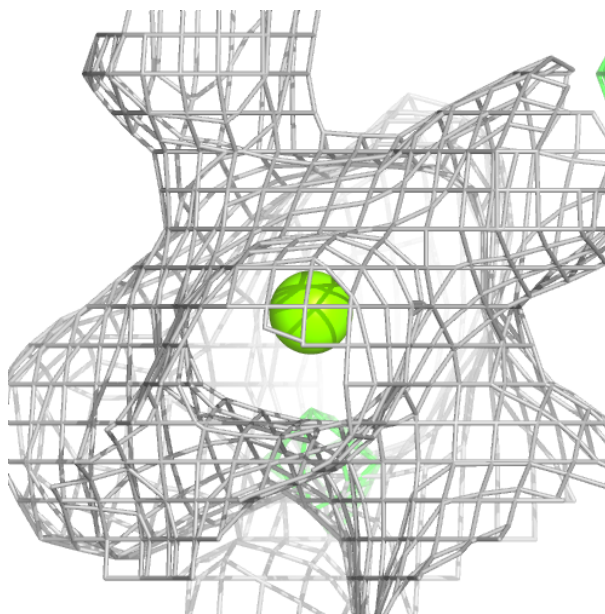
Electron density around NAD A 2101:

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



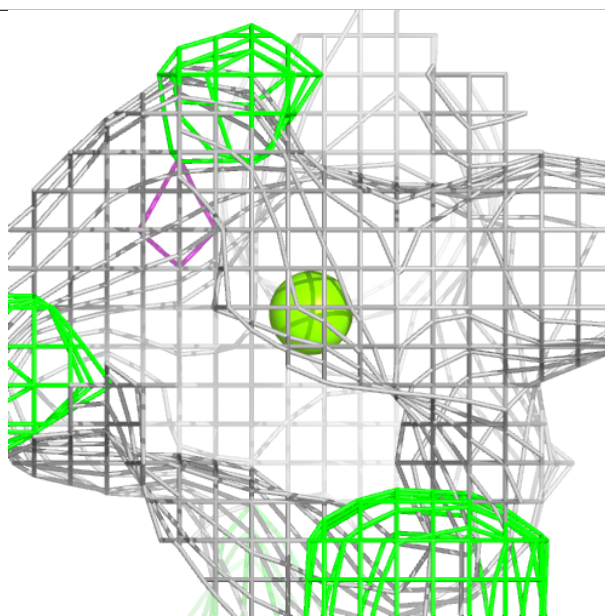
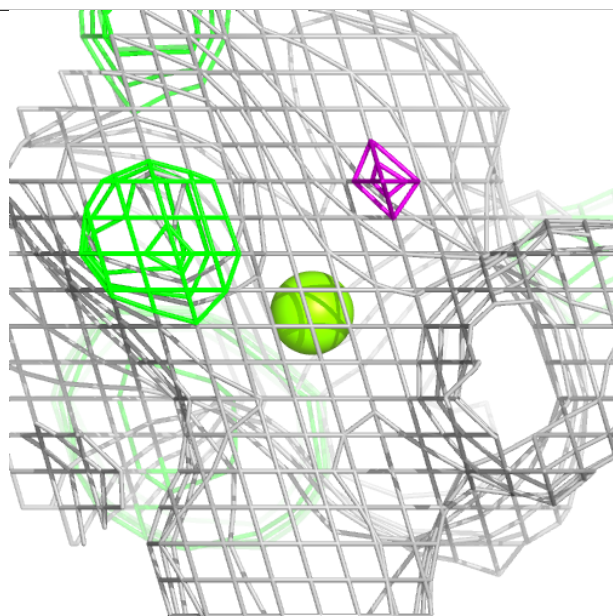
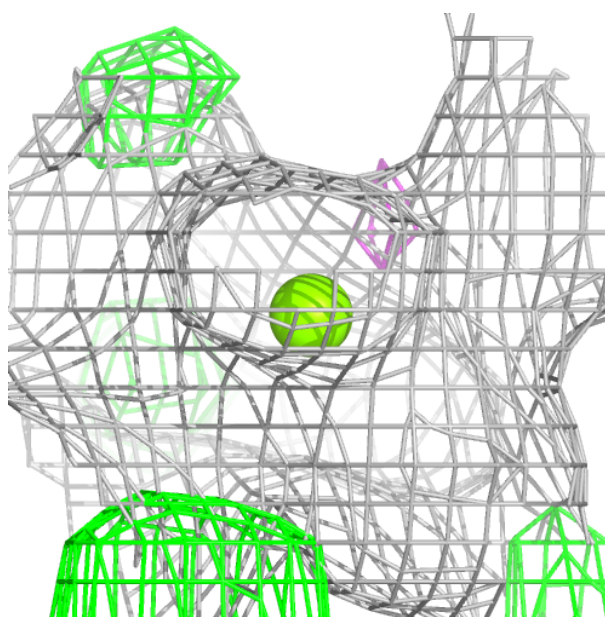
Electron density around MG A 2106:

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



Electron density around MG B 2104:

$2mF_o-DF_c$ (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.