



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 PM UTC

PDB ID : 9C8C / pdb_00009c8c
Title : Structure of proline utilization A with the FAD covalently-modified by propanal resulting from inactivation with N-allylglycine
Authors : Tanner, J.J.
Deposited on : 2024-06-12
Resolution : 1.54 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

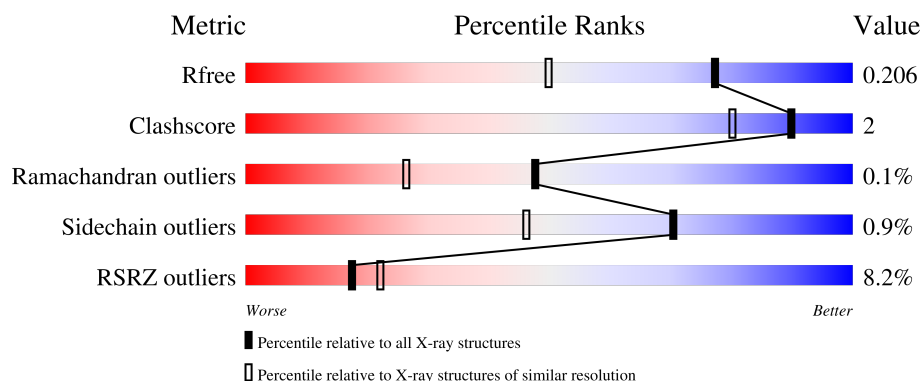
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	6% 94%
1	B	1235	10% 91% 6%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 19278 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.

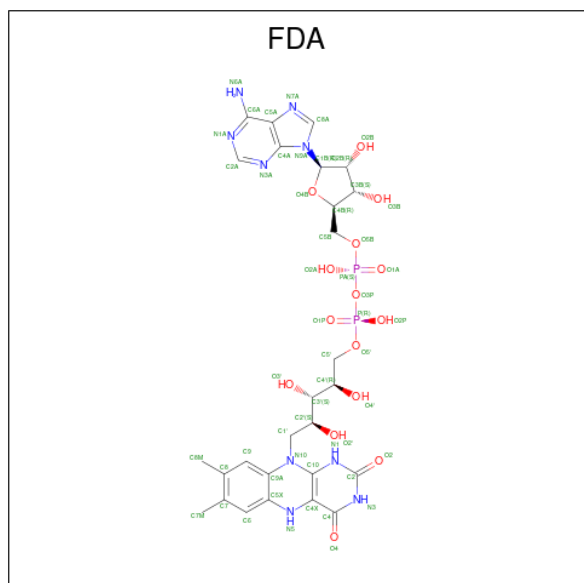
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1210	Total	C	N	O	S	0	4	0
			8880	5596	1583	1669	32			
1	B	1206	Total	C	N	O	S	0	6	0
			8832	5573	1581	1648	30			

There are 6 discrepancies between the modelled and reference sequences:

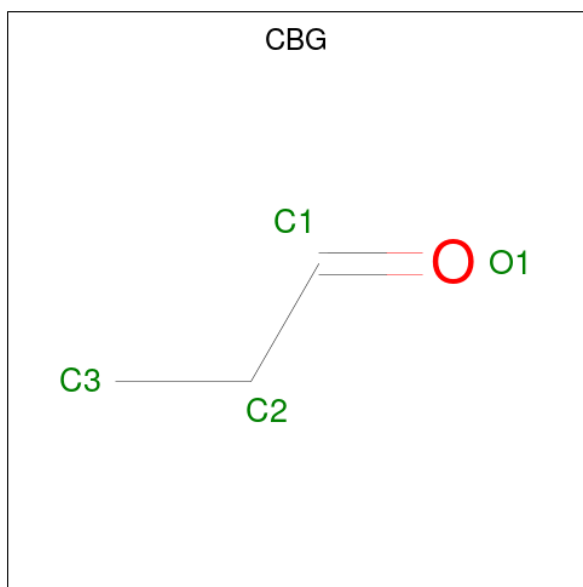
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
A	844	ALA	CYS	engineered mutation	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3
B	844	ALA	CYS	engineered mutation	UNP F7X6I3

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PROPANAL (CCD ID: CBG) (formula: C_3H_6O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

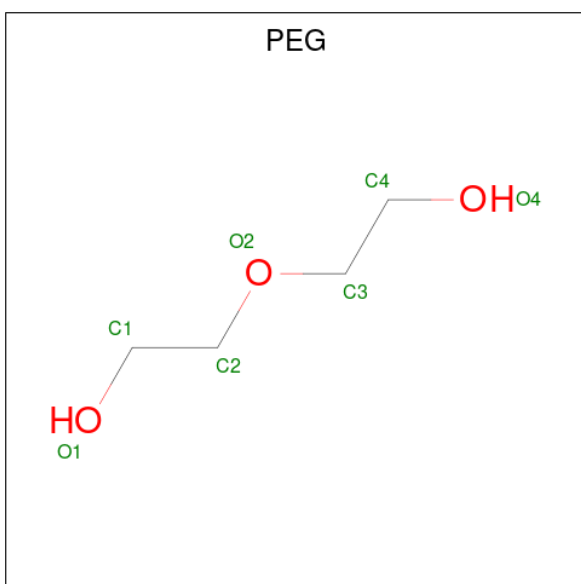
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



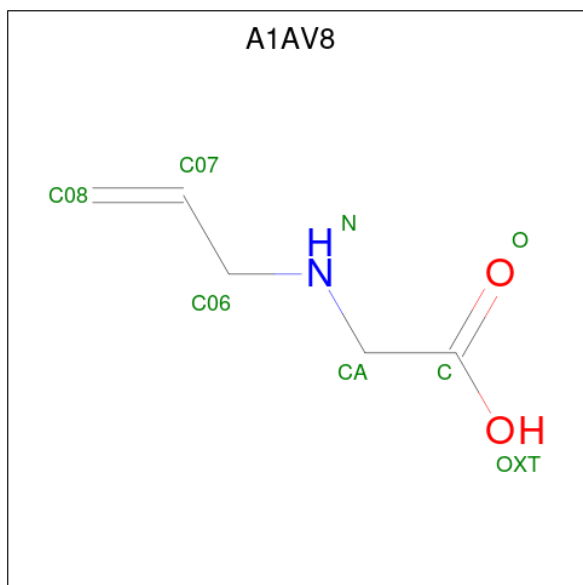
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



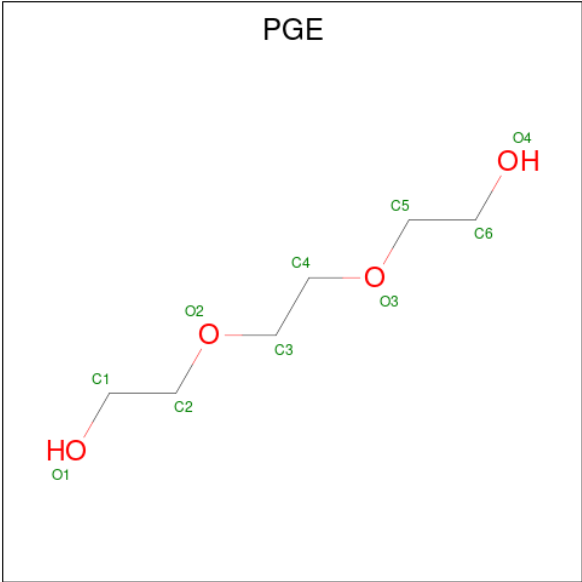
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is N-(prop-2-en-1-yl)glycine (CCD ID: A1AV8) (formula: C₅H₉NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		

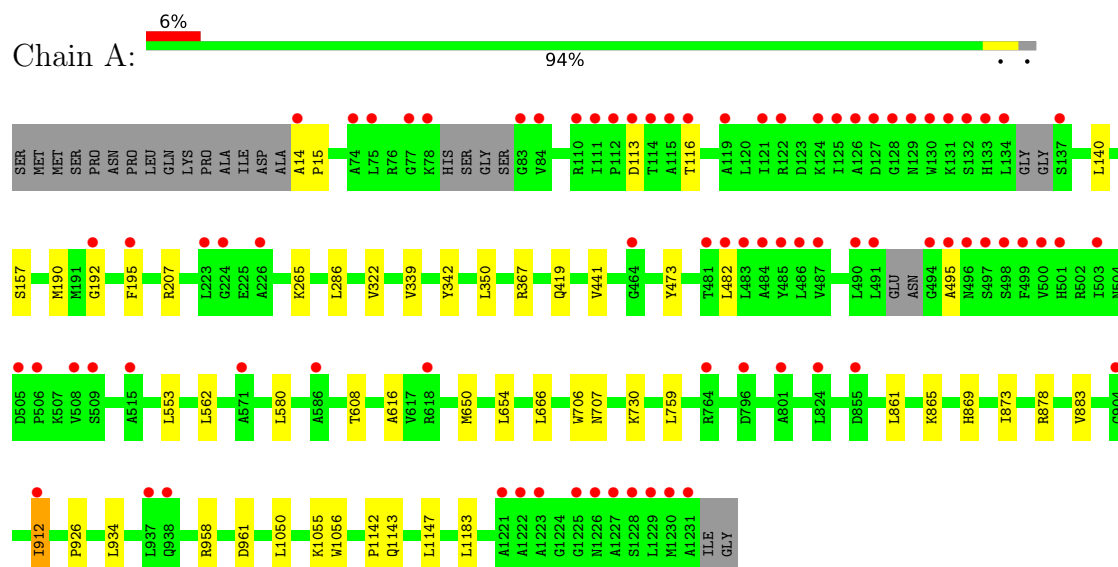
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	644	Total	O	0	0
			644	644		
10	B	654	Total	O	0	0
			654	654		

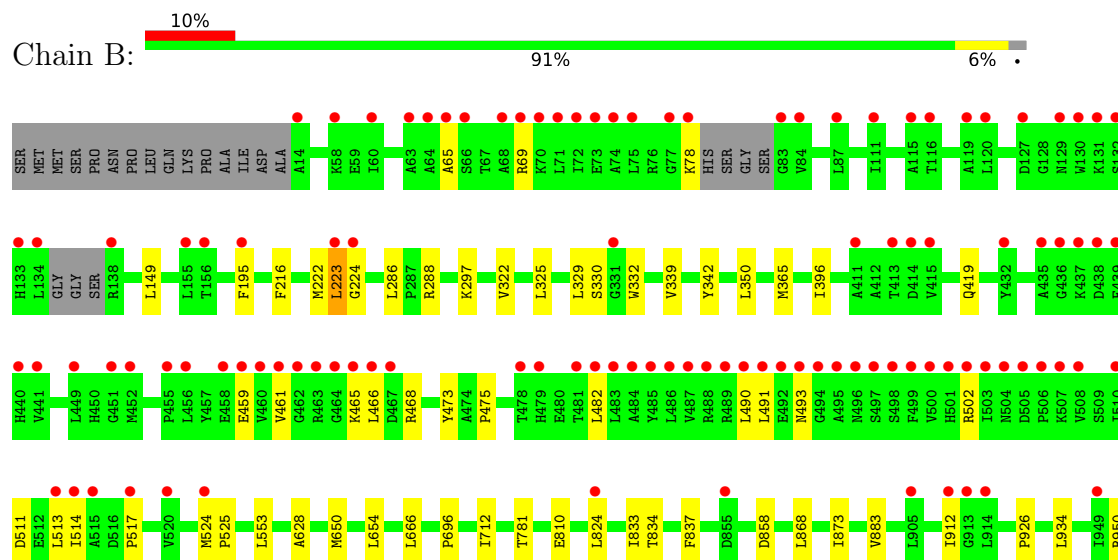
3 Residue-property plots [i](#)

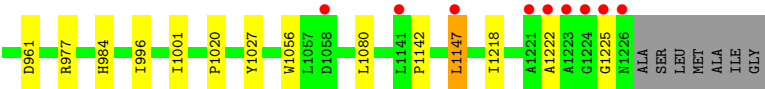
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.25Å 102.31Å 127.00Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	89.28 – 1.54 89.28 – 1.54	Depositor EDS
% Data completeness (in resolution range)	96.0 (89.28-1.54) 98.6 (89.28-1.54)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.186 , 0.205 0.189 , 0.206	Depositor DCC
R_{free} test set	17967 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.1	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	19278	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, CBG, NAD, MG, FDA, PGE, A1AV8, 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	0.26	0/9048	0.45	0/12329
1	B	0.25	0/9006	0.45	0/12278
All	All	0.26	0/18054	0.45	0/24607

There are no bond length outliers.

There are no bond angle outliers.

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	8880	0	8829	28	0
1	B	8832	0	8792	39	0
2	A	53	0	32	1	0
2	B	53	0	32	1	0
3	A	4	0	4	0	0
3	B	4	0	4	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
7	A	7	0	10	0	0
7	B	14	0	20	0	0
8	B	8	0	0	0	0
9	B	10	0	14	0	0
10	A	644	0	0	3	0
10	B	654	0	0	2	0
All	All	19278	0	17789	65	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 (65) 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:491:LEU:HD11	1:B:1225:GLY:HA3	1.70	0.73
1:B:195:PHE:HB3	1:B:482:LEU:HD11	1.78	0.66
1:A:1183:LEU:O	10:A:1401:HOH:O	2.15	0.63
1:B:858:ASP:OD1	1:B:950:ARG:NH2	2.30	0.61
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.83	0.59
1:B:650:MET:O	1:B:654:LEU:HG	2.02	0.59
1:A:650:MET:O	1:A:654:LEU:HG	2.04	0.58
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.86	0.58
1:B:873:ILE:HG13	1:B:883:VAL:HB	1.84	0.57
1:B:996[A]:ILE:HD12	1:B:1218:ILE:HG12	1.86	0.57
1:A:195:PHE:HB3	1:A:482:LEU:HD11	1.87	0.56
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.90	0.54
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.88	0.54
1:B:223:LEU:HD21	1:B:475:PRO:HB3	1.89	0.54
1:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.41	0.53
1:B:466:LEU:O	1:B:468:ARG:NH1	2.42	0.53
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.92	0.52
1:B:553:LEU:HD12	1:B:666:LEU:HD13	1.92	0.51
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.91	0.51
1:B:216:PHE:CE1	1:B:461:VAL:HG21	2.46	0.50
1:B:834:THR:HG22	1:B:1001:ILE:HD11	1.93	0.50
1:B:396:ILE:HD11	1:B:517:PRO:HA	1.94	0.49
1:A:1147:LEU:HD22	1:B:1147:LEU:HD12	1.93	0.49
1:A:869:HIS:ND1	1:A:912:ILE:HG22	2.27	0.49
1:B:459:GLU:OE1	1:B:465:LYS:NZ	2.32	0.49
1:B:69:ARG:NH1	1:B:511:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:ARG:NH2	1:B:1222:ALA:HB1	2.29	0.48
1:B:1020:PRO:HG2	1:B:1027:TYR:HA	1.95	0.48
1:B:149:LEU:HD13	1:B:490:LEU:HB2	1.96	0.48
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.96	0.48
1:B:502:ARG:HB3	1:B:513:LEU:HD21	1.97	0.47
1:B:524:MET:HE3	1:B:525:PRO:HD2	1.96	0.47
1:B:222:MET:O	1:B:224:GLY:N	2.48	0.47
1:A:473:TYR:HB2	2:A:1301:FDA:HM72	1.96	0.47
1:B:78:LYS:NZ	1:B:459:GLU:OE2	2.30	0.47
1:A:878:ARG:HD2	10:A:1717:HOH:O	2.15	0.46
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.50	0.46
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.50	0.46
1:B:65:ALA:HB1	1:B:514:ILE:HD12	1.99	0.45
1:A:912:ILE:HD11	1:A:926:PRO:HD2	1.98	0.45
1:B:912:ILE:HD11	1:B:926:PRO:HD2	1.98	0.45
1:A:608:THR:HG21	1:A:759:LEU:HD12	1.98	0.45
1:A:958:ARG:O	1:A:961:ASP:HB2	2.16	0.45
1:B:288:ARG:NH2	10:B:1412:HOH:O	2.49	0.45
1:A:1143:GLN:O	1:A:1147:LEU:HG	2.17	0.44
1:B:502:ARG:HH11	1:B:513:LEU:HD23	1.82	0.44
1:B:473:TYR:HB2	2:B:1301:FDA:HM72	2.00	0.43
1:B:837:PHE:CE2	1:B:868:LEU:HD21	2.53	0.43
1:A:113:ASP:HB3	1:A:116:THR:HG22	2.00	0.43
1:A:562:LEU:HD11	1:A:654:LEU:HD12	2.01	0.42
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.54	0.42
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.54	0.42
1:A:553:LEU:HD12	1:A:666:LEU:HD13	2.01	0.42
1:B:1080[A]:LEU:HD12	10:B:1878:HOH:O	2.19	0.42
1:B:365:MET:HE2	1:B:419:GLN:OE1	2.20	0.42
1:A:861:LEU:HG	1:A:865:LYS:HE3	2.02	0.41
1:A:192:GLY:O	1:A:207:ARG:NH1	2.54	0.41
1:A:265:LYS:HE3	10:A:1626:HOH:O	2.20	0.41
1:B:628:ALA:HB2	1:B:696:PRO:HG3	2.02	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	1.90	0.41
1:B:712:ILE:HD13	1:B:781:THR:HG21	2.03	0.40
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.03	0.40
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.46	0.40
1:A:580:LEU:CD1	1:A:616:ALA:HB2	2.52	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	1206/1235 (98%)	1180 (98%)	25 (2%)	1 (0%)	48	26
1	B	1206/1235 (98%)	1182 (98%)	22 (2%)	2 (0%)	43	25
All	All	2412/2470 (98%)	2362 (98%)	47 (2%)	3 (0%)	48	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	ALA
1	B	223	LEU
1	B	493	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	879/950 (92%)	872 (99%)	7 (1%)	73	51
1	B	869/950 (92%)	861 (99%)	8 (1%)	70	46
All	All	1748/1900 (92%)	1733 (99%)	15 (1%)	70	46

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

Mol	Chain	Res	Type
1	A	140	LEU
1	A	157	SER
1	A	342	TYR

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Mol	Chain	Res	Type
1	A	441	VAL
1	A	730	LYS
1	A	912	ILE
1	A	934	LEU
1	B	325	LEU
1	B	330	SER
1	B	342	TYR
1	B	810	GLU
1	B	824	LEU
1	B	833	ILE
1	B	934	LEU
1	B	1147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	440	HIS
1	A	501	HIS
1	A	894	ASN
1	A	1040	GLN
1	A	1114	HIS
1	B	28	GLN
1	B	426	GLN
1	B	1115	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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
8	A1AV8	B	1303	-	6,7,7	2.23	2 (33%)	5,7,7	1.07	0
4	NAD	A	1303	5	46,48,48	3.81	19 (41%)	64,73,73	2.10	16 (25%)
6	SO4	A	1305	-	4,4,4	0.54	0	6,6,6	0.26	0
3	CBG	B	1302	2	3,3,3	0.50	0	1,2,2	0.65	0
7	PEG	B	1309	-	6,6,6	0.51	0	5,5,5	0.45	0
2	FDA	B	1301	3	57,58,58	2.73	21 (36%)	78,89,89	1.92	18 (23%)
6	SO4	A	1307	-	4,4,4	0.65	0	6,6,6	0.18	0
6	SO4	B	1306	-	4,4,4	0.61	0	6,6,6	0.07	0
6	SO4	A	1306	-	4,4,4	0.71	0	6,6,6	0.23	0
6	SO4	A	1308	-	4,4,4	0.68	0	6,6,6	0.09	0
7	PEG	B	1308	-	6,6,6	0.46	0	5,5,5	0.30	0
9	PGE	B	1307	-	9,9,9	0.54	0	8,8,8	0.22	0
4	NAD	B	1304	5	46,48,48	3.50	19 (41%)	64,73,73	2.08	12 (18%)
7	PEG	A	1309	-	6,6,6	0.50	0	5,5,5	0.17	0
3	CBG	A	1302	2	3,3,3	0.52	0	1,2,2	0.66	0
2	FDA	A	1301	3	57,58,58	2.81	22 (38%)	78,89,89	1.92	18 (23%)

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
8	A1AV8	B	1303	-	-	1/5/5/5	-
4	NAD	A	1303	5	-	5/30/62/62	0/5/5/5
3	CBG	B	1302	2	-	0/0/1/1	-
7	PEG	B	1309	-	-	0/4/4/4	-
2	FDA	B	1301	3	-	6/34/50/50	0/6/6/6
7	PEG	B	1308	-	-	2/4/4/4	-
9	PGE	B	1307	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	B	1304	5	-	3/30/62/62	0/5/5/5
7	PEG	A	1309	-	-	1/4/4/4	-
3	CBG	A	1302	2	-	0/0/1/1	-
2	FDA	A	1301	3	-	6/34/50/50	0/6/6/6

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1303	NAD	O4D-C1D	-9.77	1.28	1.40
2	A	1301	FDA	PA-O3P	-9.53	1.49	1.59
4	A	1303	NAD	PN-O3	9.17	1.69	1.59
2	B	1301	FDA	PA-O3P	-9.02	1.49	1.59
4	A	1303	NAD	C3B-C4B	-8.79	1.30	1.53
4	B	1304	NAD	O4D-C1D	-8.67	1.29	1.40
4	B	1304	NAD	C3B-C4B	-8.34	1.31	1.53
4	B	1304	NAD	C3D-C4D	-8.05	1.32	1.53
4	A	1303	NAD	C7N-N7N	7.86	1.47	1.33
4	A	1303	NAD	C3D-C4D	-7.81	1.33	1.53
4	B	1304	NAD	C7N-N7N	7.72	1.47	1.33
4	A	1303	NAD	O4B-C4B	7.33	1.61	1.45
4	B	1304	NAD	O4D-C4D	7.30	1.61	1.45
2	B	1301	FDA	O4-C4	7.26	1.37	1.23
4	A	1303	NAD	O4D-C4D	7.24	1.61	1.45
2	A	1301	FDA	O4-C4	7.17	1.37	1.23
4	B	1304	NAD	O4B-C4B	6.88	1.60	1.45
4	B	1304	NAD	PN-O3	6.61	1.66	1.59
2	A	1301	FDA	C6-C5X	6.19	1.49	1.39
2	B	1301	FDA	C6-C5X	6.11	1.49	1.39
2	B	1301	FDA	O2-C2	6.06	1.36	1.23
4	B	1304	NAD	C6A-N6A	5.90	1.49	1.34
2	A	1301	FDA	O2-C2	5.63	1.35	1.23
4	A	1303	NAD	C6A-N6A	5.57	1.48	1.34
2	A	1301	FDA	C9-C9A	5.50	1.48	1.39
2	A	1301	FDA	P-O3P	5.37	1.65	1.59
2	B	1301	FDA	C9-C9A	4.82	1.47	1.39
4	A	1303	NAD	PA-O3	4.54	1.64	1.59
2	A	1301	FDA	C4X-N5	4.45	1.44	1.35
2	B	1301	FDA	C4X-N5	4.39	1.44	1.35
2	B	1301	FDA	C5X-C9A	-4.24	1.35	1.40
2	A	1301	FDA	C5X-N5	4.20	1.47	1.39
8	B	1303	A1AV8	CA-C	4.07	1.60	1.50
4	A	1303	NAD	O3D-C3D	4.03	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1304	NAD	C3N-C7N	3.95	1.56	1.50
2	B	1301	FDA	C10-N1	3.94	1.44	1.37
2	B	1301	FDA	P-O3P	3.86	1.63	1.59
4	A	1303	NAD	O4B-C1B	-3.81	1.33	1.42
2	B	1301	FDA	C2-N1	3.80	1.43	1.37
2	A	1301	FDA	C6A-N6A	3.79	1.43	1.34
2	B	1301	FDA	C6A-N6A	3.75	1.43	1.34
4	A	1303	NAD	C3N-C7N	3.64	1.56	1.50
2	A	1301	FDA	C10-N1	3.61	1.43	1.37
4	B	1304	NAD	O3D-C3D	3.55	1.51	1.43
2	A	1301	FDA	C2-N1	3.50	1.43	1.37
4	A	1303	NAD	C2N-N1N	3.06	1.38	1.35
2	B	1301	FDA	C5X-N5	3.03	1.45	1.39
4	A	1303	NAD	O3B-C3B	3.02	1.50	1.43
4	A	1303	NAD	O7N-C7N	-3.01	1.18	1.24
4	B	1304	NAD	C2N-N1N	2.98	1.38	1.35
4	B	1304	NAD	O7N-C7N	-2.91	1.18	1.24
4	B	1304	NAD	O4B-C1B	-2.84	1.35	1.42
2	A	1301	FDA	C5X-C9A	-2.83	1.37	1.40
4	B	1304	NAD	O3B-C3B	2.83	1.50	1.43
4	B	1304	NAD	C2A-N1A	2.78	1.38	1.33
2	A	1301	FDA	C4X-C4	2.77	1.50	1.41
2	A	1301	FDA	PA-O5B	-2.76	1.48	1.59
2	A	1301	FDA	O2'-C2'	-2.70	1.37	1.43
4	A	1303	NAD	C5A-C4A	-2.60	1.34	1.39
4	A	1303	NAD	C8A-N9A	-2.59	1.33	1.37
2	B	1301	FDA	C4X-C4	2.58	1.49	1.41
2	B	1301	FDA	C10-N10	2.57	1.42	1.38
8	B	1303	A1AV8	O-C	2.55	1.30	1.22
2	A	1301	FDA	C10-N10	2.54	1.42	1.38
4	A	1303	NAD	C2A-N1A	2.54	1.38	1.33
4	A	1303	NAD	O2B-C2B	-2.43	1.36	1.43
2	B	1301	FDA	C9A-N10	2.35	1.45	1.41
2	B	1301	FDA	P-O1P	2.32	1.58	1.50
4	B	1304	NAD	C8A-N7A	2.24	1.36	1.31
2	B	1301	FDA	PA-O5B	-2.23	1.50	1.59
2	A	1301	FDA	C2-N3	2.22	1.41	1.37
2	B	1301	FDA	O3B-C3B	-2.20	1.37	1.43
2	A	1301	FDA	C5A-C4A	2.17	1.43	1.39
2	B	1301	FDA	C5A-C4A	2.17	1.43	1.39
4	B	1304	NAD	C5A-N7A	-2.16	1.35	1.39
2	A	1301	FDA	C9-C8	2.16	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1304	NAD	PA-O5B	2.15	1.67	1.59
2	A	1301	FDA	O3B-C3B	-2.13	1.37	1.43
4	B	1304	NAD	C5A-C4A	-2.10	1.35	1.39
2	B	1301	FDA	C2A-N3A	2.05	1.37	1.33
2	A	1301	FDA	P-O1P	2.05	1.57	1.50
2	B	1301	FDA	C4A-N9A	2.03	1.41	1.37
2	A	1301	FDA	C9A-N10	2.01	1.44	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1304	NAD	N3A-C2A-N1A	-6.04	119.43	128.58
4	B	1304	NAD	C5A-C4A-N3A	-6.03	118.41	126.72
4	A	1303	NAD	C4A-N9A-C1B	-5.69	113.33	126.63
4	A	1303	NAD	N3A-C2A-N1A	-5.63	120.06	128.58
2	B	1301	FDA	N3A-C2A-N1A	-5.49	120.27	128.58
2	A	1301	FDA	N3A-C2A-N1A	-5.49	120.28	128.58
2	A	1301	FDA	C5A-C4A-N3A	-5.28	119.44	126.72
4	B	1304	NAD	N9A-C8A-N7A	-5.23	106.52	113.94
4	A	1303	NAD	C5A-C4A-N3A	-5.13	119.65	126.72
4	A	1303	NAD	N9A-C8A-N7A	-5.12	106.67	113.94
2	B	1301	FDA	O2A-PA-O3P	4.91	120.54	107.27
4	B	1304	NAD	C4A-N9A-C1B	-4.83	115.34	126.63
4	B	1304	NAD	N3A-C4A-N9A	4.76	135.27	127.17
2	B	1301	FDA	O3P-PA-O1A	-4.72	96.51	110.70
2	A	1301	FDA	O3P-PA-O1A	-4.71	96.52	110.70
2	B	1301	FDA	C5A-C4A-N3A	-4.68	120.28	126.72
2	A	1301	FDA	N3A-C4A-N9A	4.48	134.78	127.17
2	A	1301	FDA	O2A-PA-O3P	4.44	119.28	107.27
4	A	1303	NAD	C1B-N9A-C8A	4.43	136.93	127.09
2	A	1301	FDA	C4-N3-C2	-4.42	120.29	126.37
4	B	1304	NAD	C2A-N3A-C4A	4.18	122.03	111.83
2	B	1301	FDA	C4-N3-C2	-4.11	120.71	126.37
2	B	1301	FDA	N3-C2-N1	4.10	122.19	115.74
2	B	1301	FDA	N3A-C4A-N9A	4.02	134.01	127.17
2	B	1301	FDA	C5A-N7A-C8A	3.91	109.59	103.45
2	A	1301	FDA	C5A-N7A-C8A	3.82	109.45	103.45
4	A	1303	NAD	N3A-C4A-N9A	3.81	133.65	127.17
4	A	1303	NAD	C4A-N9A-C8A	3.80	109.73	105.74
4	B	1304	NAD	C4A-N9A-C8A	3.78	109.71	105.74
2	A	1301	FDA	N3-C2-N1	3.66	121.49	115.74
4	A	1303	NAD	C2N-C3N-C4N	3.65	122.50	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1303	NAD	C4D-O4D-C1D	-3.59	106.64	109.92
2	A	1301	FDA	C2A-N3A-C4A	3.57	120.55	111.83
4	B	1304	NAD	C1B-N9A-C8A	3.54	134.95	127.09
4	A	1303	NAD	C5A-N7A-C8A	3.53	109.00	103.45
4	A	1303	NAD	C2A-N3A-C4A	3.42	120.18	111.83
4	B	1304	NAD	C5A-N7A-C8A	3.40	108.79	103.45
2	A	1301	FDA	N9A-C8A-N7A	-3.34	109.19	113.94
2	B	1301	FDA	N9A-C8A-N7A	-3.33	109.22	113.94
2	B	1301	FDA	C2A-N3A-C4A	3.19	119.62	111.83
4	B	1304	NAD	C6N-N1N-C2N	-3.13	119.21	121.88
4	B	1304	NAD	C2N-C3N-C4N	3.12	121.89	118.26
2	B	1301	FDA	C4A-C5A-N7A	-3.00	107.15	110.58
4	B	1304	NAD	C4D-O4D-C1D	-2.92	107.25	109.92
2	A	1301	FDA	C4A-C5A-N7A	-2.67	107.52	110.58
2	A	1301	FDA	C4X-C4-N3	2.57	119.19	112.13
2	B	1301	FDA	C4A-N9A-C8A	2.46	108.33	105.74
4	A	1303	NAD	C4A-C5A-N7A	-2.34	107.90	110.58
2	B	1301	FDA	O3P-P-O1P	2.33	117.72	110.70
2	A	1301	FDA	C5X-N5-C4X	-2.31	115.75	121.08
2	B	1301	FDA	O5B-PA-O1A	-2.30	99.81	108.94
2	A	1301	FDA	O5B-PA-O1A	-2.28	99.88	108.94
2	B	1301	FDA	C5X-N5-C4X	-2.21	115.98	121.08
4	A	1303	NAD	C6N-N1N-C2N	-2.21	120.00	121.88
2	A	1301	FDA	C4A-N9A-C8A	2.20	108.05	105.74
2	B	1301	FDA	C9-C9A-N10	-2.19	118.91	121.85
4	A	1303	NAD	C5N-C4N-C3N	-2.17	118.23	120.36
2	B	1301	FDA	C4X-C4-N3	2.15	118.02	112.13
2	B	1301	FDA	C2A-N1A-C6A	2.14	122.25	118.73
2	A	1301	FDA	C9A-C5X-N5	2.13	121.97	119.37
4	A	1303	NAD	C2D-C3D-C4D	2.08	106.63	102.61
2	A	1301	FDA	O5'-P-O1P	2.06	117.12	108.94
4	A	1303	NAD	O2N-PN-O3	2.03	112.76	107.27
2	A	1301	FDA	C4-C4X-N5	2.01	121.51	116.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	FDA	C2'-C3'-C4'-C5'
2	B	1301	FDA	C2'-C3'-C4'-O4'
2	A	1301	FDA	C2'-C3'-C4'-O4'
4	A	1303	NAD	C3D-C4D-C5D-O5D

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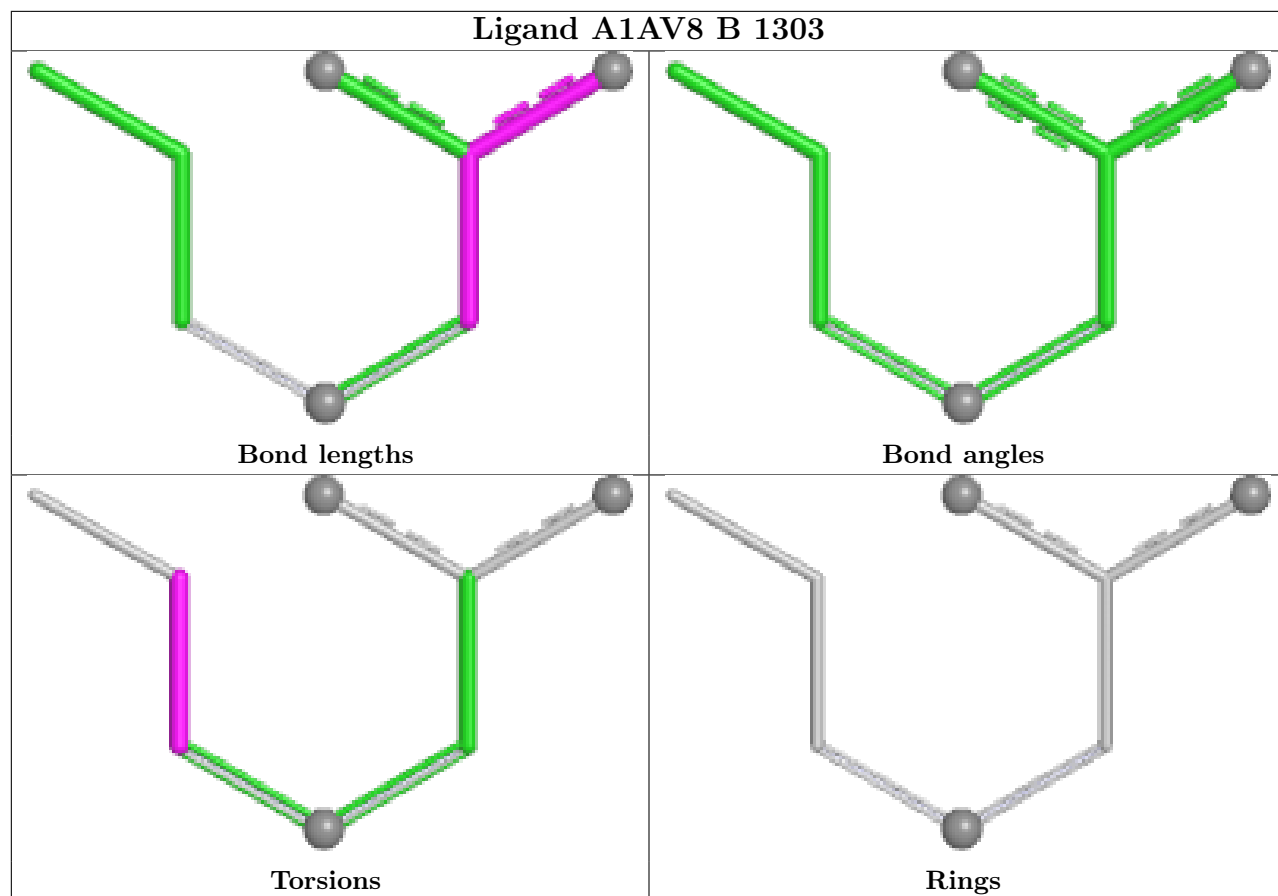
Mol	Chain	Res	Type	Atoms
2	A	1301	FDA	PA-O3P-P-O1P
2	B	1301	FDA	PA-O3P-P-O1P
4	A	1303	NAD	O4D-C4D-C5D-O5D
7	A	1309	PEG	O1-C1-C2-O2
2	B	1301	FDA	O3'-C3'-C4'-C5'
7	B	1308	PEG	C1-C2-O2-C3
4	A	1303	NAD	C2B-C1B-N9A-C8A
4	B	1304	NAD	C2B-C1B-N9A-C8A
2	B	1301	FDA	O3'-C3'-C4'-O4'
4	A	1303	NAD	C5B-O5B-PA-O1A
4	A	1303	NAD	C4D-C5D-O5D-PN
2	A	1301	FDA	PA-O3P-P-O2P
2	B	1301	FDA	PA-O3P-P-O2P
2	A	1301	FDA	O3'-C3'-C4'-O4'
7	B	1308	PEG	C4-C3-O2-C2
2	A	1301	FDA	C2'-C3'-C4'-C5'
8	B	1303	A1AV8	N-C06-C07-C08
2	A	1301	FDA	O3'-C3'-C4'-C5'
4	B	1304	NAD	O4B-C1B-N9A-C8A
4	B	1304	NAD	C2B-C1B-N9A-C4A

There are no ring outliers.

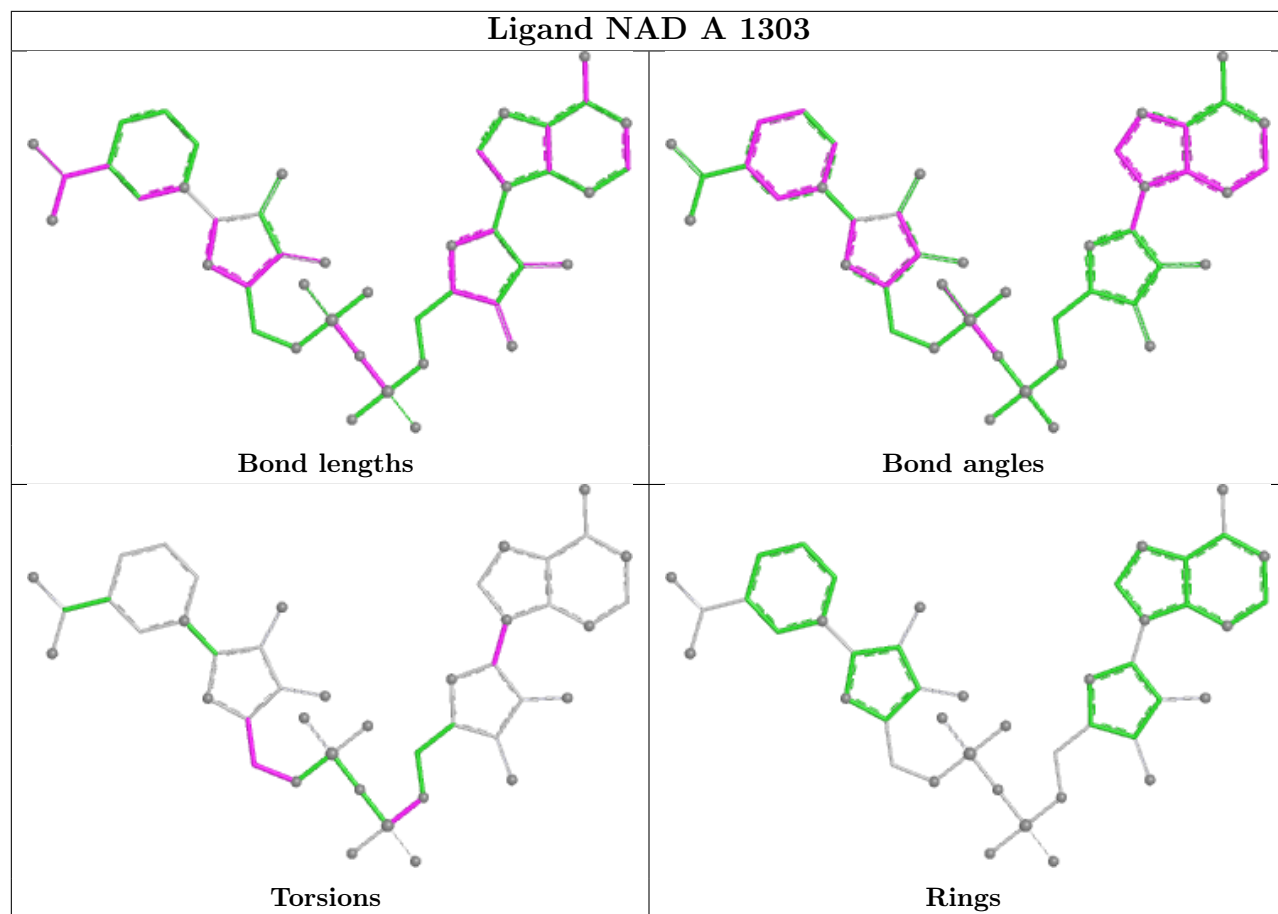
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	FDA	1	0
2	A	1301	FDA	1	0

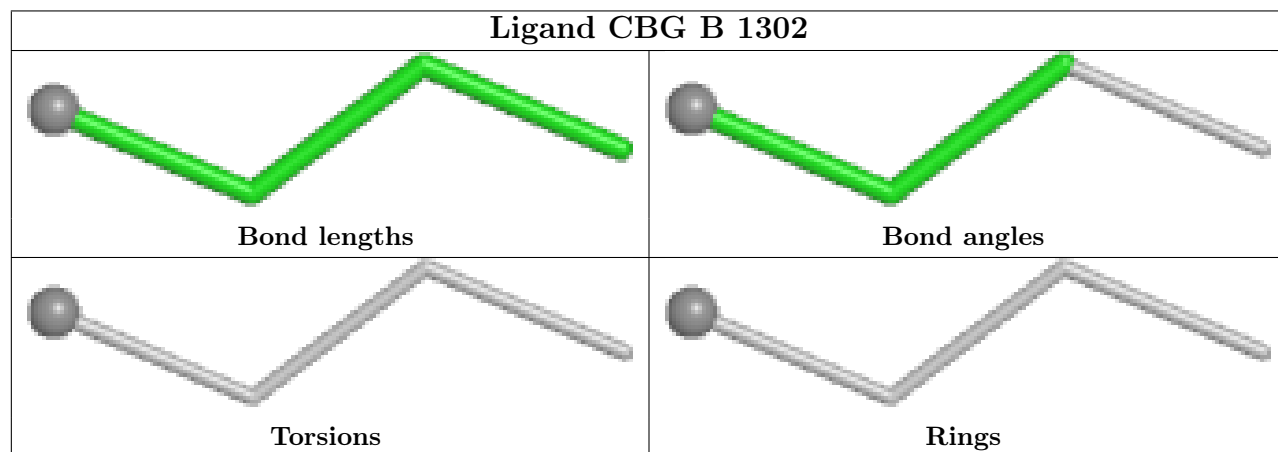
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

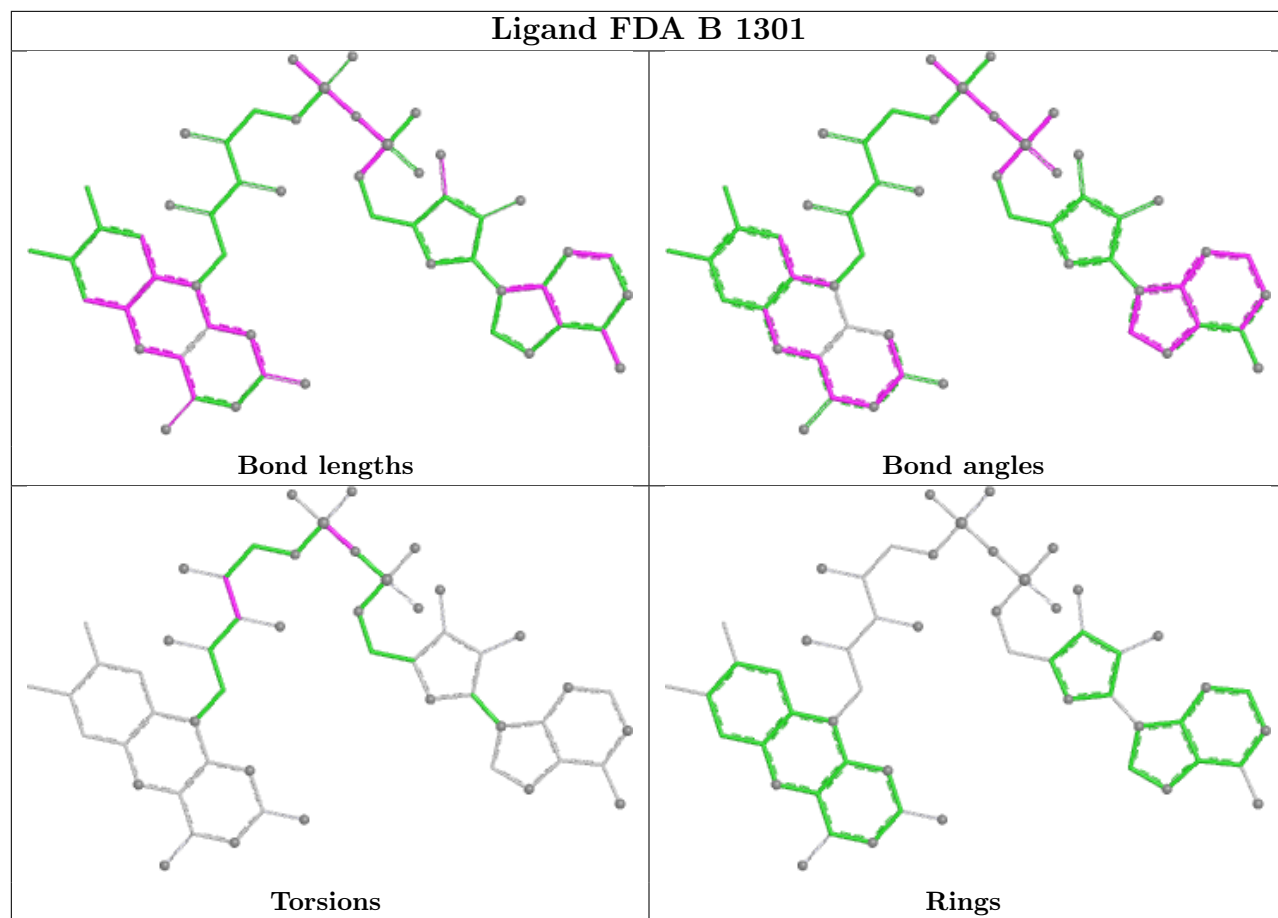


Ligand NAD A 1303

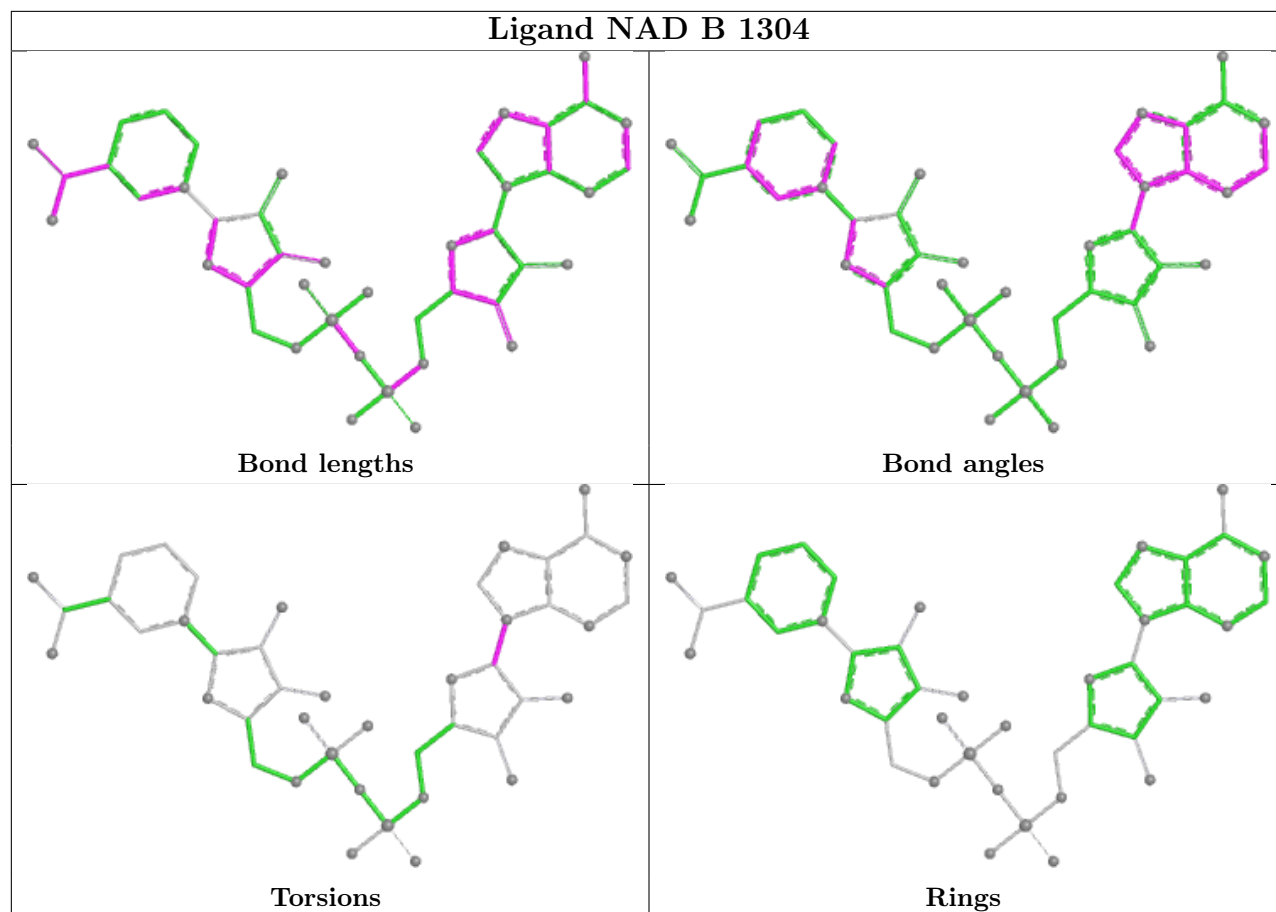


Ligand CBG B 1302

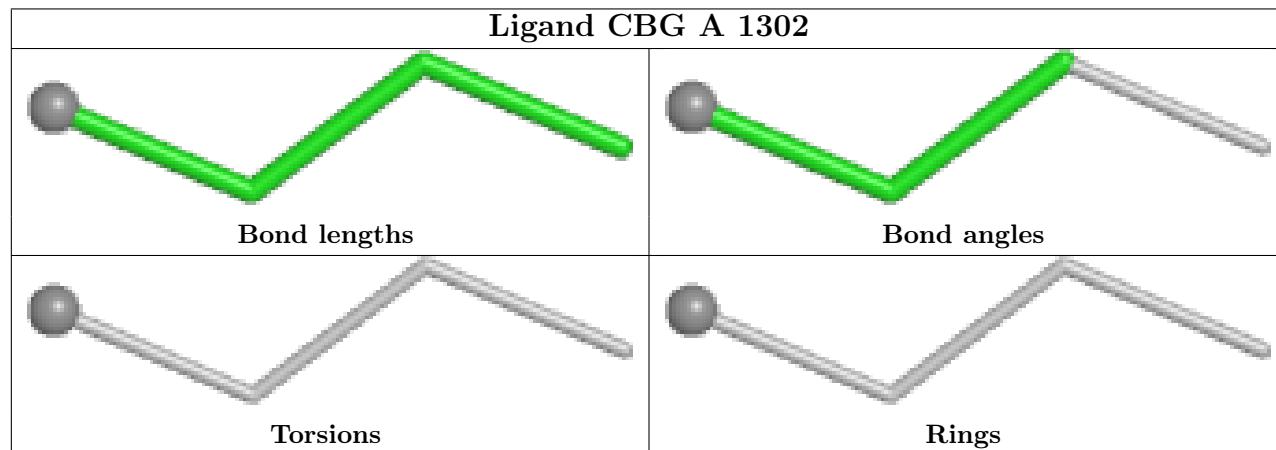


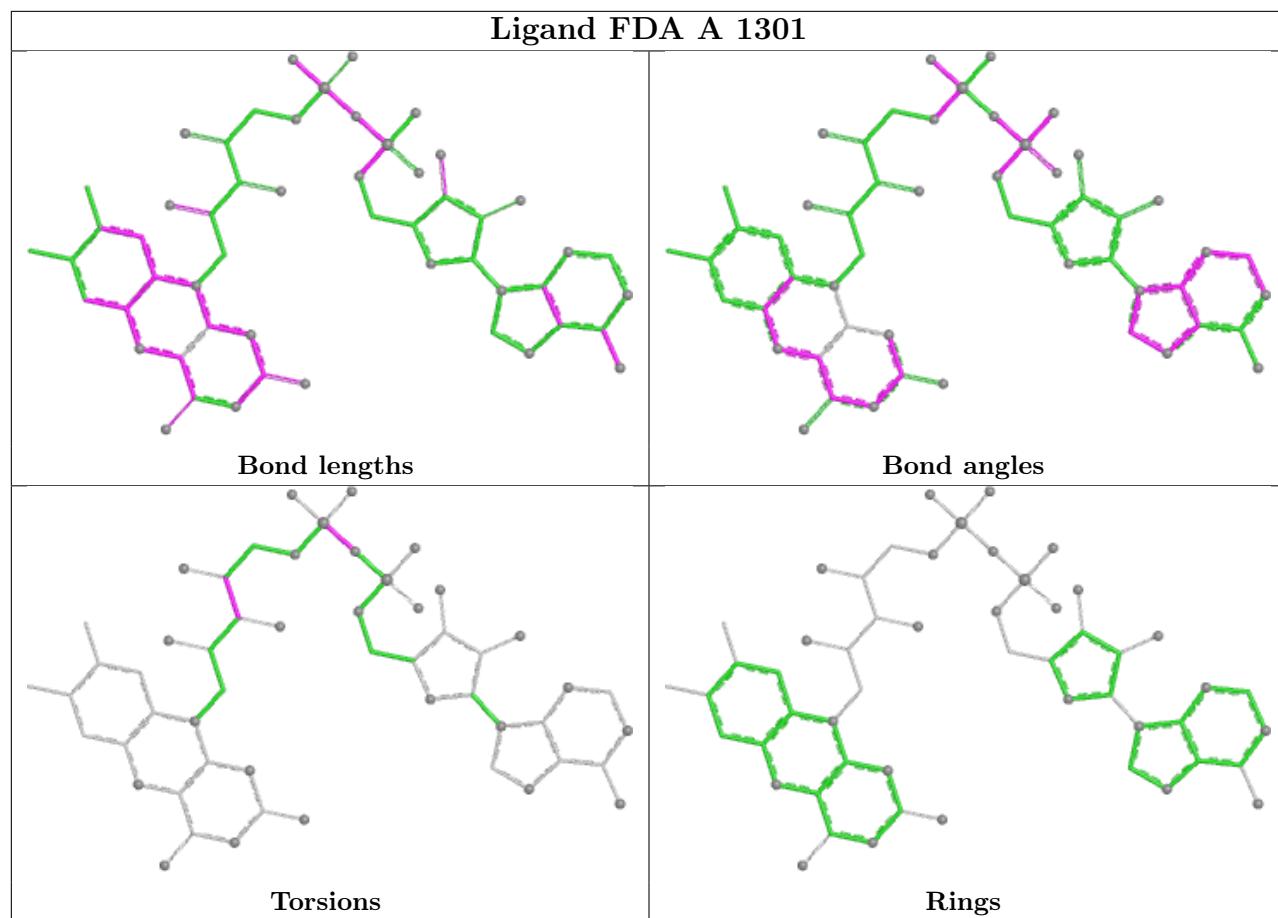


Ligand NAD B 1304



Ligand CBG A 1302





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%)	0.38	80 (6%) 24 30	13, 27, 49, 80	4 (0%)
1	B	1206/1235 (97%)	0.52	119 (9%) 13 17	12, 27, 53, 82	6 (0%)
All	All	2416/2470 (97%)	0.45	199 (8%) 17 22	12, 27, 52, 82	10 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1222	ALA	7.5
1	B	485	TYR	6.6
1	B	487	VAL	6.1
1	A	503	ILE	5.6
1	B	495	ALA	5.5
1	B	439	PHE	5.4
1	B	1223	ALA	5.1
1	A	491	LEU	5.0
1	B	508	VAL	4.9
1	B	500	VAL	4.8
1	B	462	GLY	4.7
1	A	1222	ALA	4.7
1	B	481	THR	4.5
1	B	494	GLY	4.4
1	A	14	ALA	4.4
1	B	513	LEU	4.4
1	A	134	LEU	4.3
1	B	491	LEU	4.3
1	B	496	ASN	4.3
1	B	490	LEU	4.3
1	A	1231	ALA	4.3
1	A	132	SER	4.2
1	A	129	ASN	4.2
1	B	14	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	74	ALA	4.2
1	A	490	LEU	4.1
1	A	485	TYR	4.1
1	A	494	GLY	4.1
1	A	496	ASN	4.1
1	B	503	ILE	4.1
1	B	484	ALA	4.0
1	A	500	VAL	3.9
1	A	508	VAL	3.9
1	B	129	ASN	3.9
1	B	493	ASN	3.9
1	A	1223	ALA	3.9
1	B	497	SER	3.8
1	A	224	GLY	3.8
1	B	75	LEU	3.7
1	A	137	SER	3.7
1	B	461	VAL	3.7
1	B	486	LEU	3.7
1	A	130	TRP	3.7
1	B	456	LEU	3.6
1	B	132	SER	3.6
1	A	486	LEU	3.6
1	B	499	PHE	3.6
1	A	1227	ALA	3.6
1	B	133	HIS	3.5
1	B	223	LEU	3.5
1	B	72	ILE	3.5
1	B	514	ILE	3.5
1	A	1230	MET	3.5
1	A	1228	SER	3.5
1	A	482	LEU	3.5
1	B	440	HIS	3.5
1	A	115	ALA	3.5
1	B	1225	GLY	3.4
1	A	484	ALA	3.4
1	B	912	ILE	3.4
1	B	195	PHE	3.4
1	B	1226	ASN	3.4
1	A	506	PRO	3.4
1	B	77	GLY	3.4
1	B	506	PRO	3.4
1	A	127	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	463	ARG	3.4
1	B	415	VAL	3.3
1	A	495	ALA	3.3
1	B	134	LEU	3.3
1	A	1229	LEU	3.2
1	B	83	GLY	3.2
1	A	483	LEU	3.2
1	B	460	VAL	3.2
1	A	801	ALA	3.2
1	B	510	ILE	3.2
1	B	414	ASP	3.1
1	A	125	ILE	3.1
1	B	68	ALA	3.1
1	B	441	VAL	3.0
1	B	438	ASP	3.0
1	A	192	GLY	3.0
1	A	499	PHE	3.0
1	A	1226	ASN	3.0
1	B	115	ALA	3.0
1	B	464	GLY	2.9
1	B	70	LYS	2.9
1	A	223	LEU	2.9
1	B	63	ALA	2.9
1	B	224	GLY	2.9
1	B	467	ASP	2.9
1	A	796	ASP	2.8
1	B	1221	ALA	2.8
1	B	501	HIS	2.8
1	B	498	SER	2.8
1	B	127	ASP	2.8
1	B	65	ALA	2.8
1	B	458	GLU	2.8
1	A	131	LYS	2.8
1	A	122	ARG	2.8
1	B	466	LEU	2.8
1	B	413	THR	2.8
1	B	515	ALA	2.7
1	B	524	MET	2.7
1	B	489	ARG	2.7
1	B	451	GLY	2.7
1	A	78	LYS	2.7
1	A	501	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	112	PRO	2.7
1	B	436	GLY	2.7
1	A	114	THR	2.7
1	A	764	ARG	2.7
1	B	71	LEU	2.6
1	B	482	LEU	2.6
1	A	487	VAL	2.6
1	A	904	GLY	2.6
1	B	432	TYR	2.6
1	B	465	LYS	2.6
1	B	492	GLU	2.6
1	A	83	GLY	2.6
1	A	128	GLY	2.6
1	A	111	ILE	2.6
1	B	84	VAL	2.6
1	B	130	TRP	2.5
1	B	478	THR	2.5
1	B	87	LEU	2.5
1	B	156	THR	2.5
1	B	459	GLU	2.5
1	A	124	LYS	2.5
1	B	138	ARG	2.5
1	B	505	ASP	2.5
1	B	507	LYS	2.5
1	A	116	THR	2.5
1	A	126	ALA	2.4
1	B	64	ALA	2.4
1	A	497	SER	2.4
1	B	455	PRO	2.4
1	B	1147	LEU	2.4
1	A	481	THR	2.4
1	B	116	THR	2.4
1	B	155	LEU	2.4
1	B	437	LYS	2.4
1	B	449	LEU	2.4
1	B	66	SER	2.4
1	B	452	MET	2.4
1	A	195	PHE	2.4
1	A	84	VAL	2.3
1	B	479	HIS	2.3
1	A	618	ARG	2.3
1	A	498	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	113	ASP	2.3
1	B	1058	ASP	2.3
1	A	855	ASP	2.3
1	B	331	GLY	2.3
1	A	937	LEU	2.3
1	B	120	LEU	2.3
1	B	78	LYS	2.3
1	A	571	ALA	2.3
1	A	586	ALA	2.3
1	B	855	ASP	2.3
1	A	1225	GLY	2.3
1	A	912	ILE	2.3
1	B	111	ILE	2.3
1	B	1141	LEU	2.2
1	B	60	ILE	2.2
1	A	119	ALA	2.2
1	A	505	ASP	2.2
1	A	515	ALA	2.2
1	B	411	ALA	2.2
1	A	133	HIS	2.2
1	B	913	GLY	2.2
1	B	949	ILE	2.2
1	B	435	ALA	2.2
1	A	464	GLY	2.2
1	A	938	GLN	2.2
1	B	504	ASN	2.2
1	A	75	LEU	2.1
1	B	914	LEU	2.1
1	B	488	ARG	2.1
1	B	73	GLU	2.1
1	A	74	ALA	2.1
1	A	824	LEU	2.1
1	B	483	LEU	2.1
1	B	905	LEU	2.1
1	A	121	ILE	2.1
1	A	77	GLY	2.1
1	B	119	ALA	2.1
1	B	824	LEU	2.1
1	B	69	ARG	2.1
1	B	502	ARG	2.1
1	B	517	PRO	2.1
1	B	58	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	520	VAL	2.0
1	A	226	ALA	2.0
1	A	1221	ALA	2.0
1	A	110	ARG	2.0
1	B	1224	GLY	2.0
1	B	131	LYS	2.0
1	A	509	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

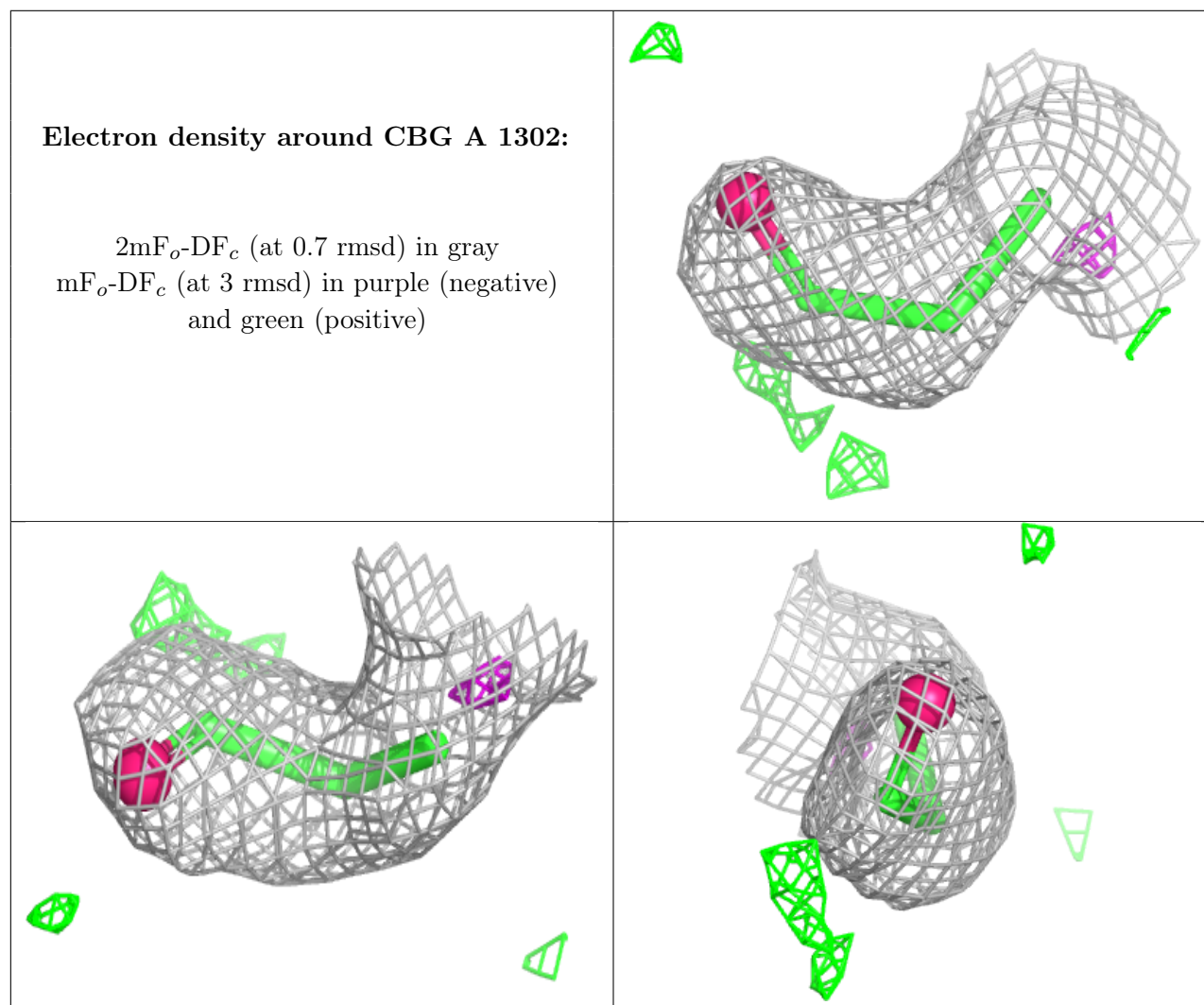
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CBG	A	1302	4/4	0.75	0.19	25,27,31,33	4
6	SO4	A	1308	5/5	0.80	0.18	49,50,51,59	5
7	PEG	B	1308	7/7	0.83	0.13	34,36,41,43	0
3	CBG	B	1302	4/4	0.84	0.17	28,28,31,35	4
6	SO4	A	1306	5/5	0.89	0.10	45,45,50,54	0
7	PEG	A	1309	7/7	0.90	0.11	30,33,43,46	0
6	SO4	A	1307	5/5	0.90	0.12	31,32,40,44	5
7	PEG	B	1309	7/7	0.92	0.11	27,29,35,41	0
9	PGE	B	1307	10/10	0.92	0.10	31,35,40,40	0
5	MG	A	1304	1/1	0.93	0.09	37,37,37,37	0
8	A1AV8	B	1303	8/8	0.93	0.10	23,27,27,29	0
4	NAD	A	1303	44/44	0.93	0.09	21,30,33,35	0
2	FDA	A	1301	53/53	0.95	0.08	22,28,32,36	0
2	FDA	B	1301	53/53	0.95	0.08	23,27,33,35	0
4	NAD	B	1304	44/44	0.96	0.07	20,24,27,28	0
5	MG	B	1305	1/1	0.98	0.06	26,26,26,26	0

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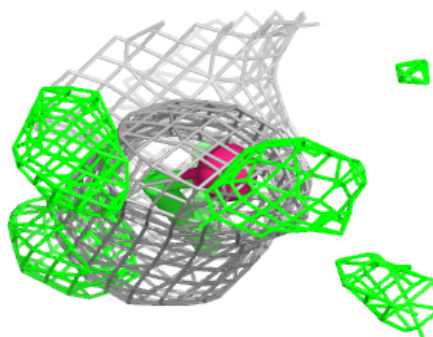
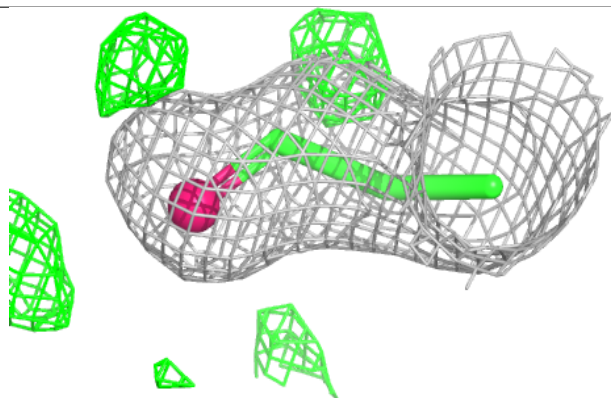
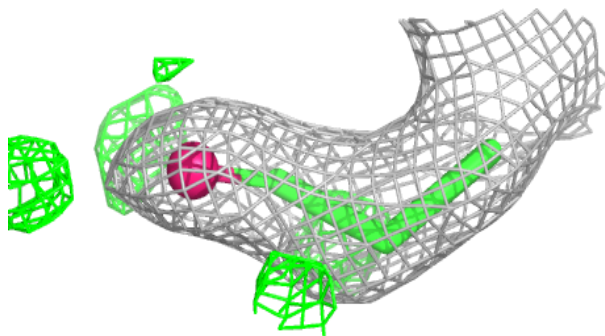
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	1306	5/5	0.99	0.05	21,21,25,26	0
6	SO4	A	1305	5/5	0.99	0.04	23,25,26,26	0

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.

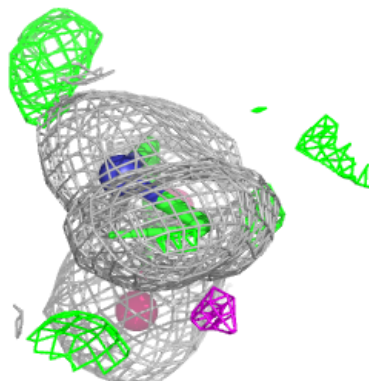
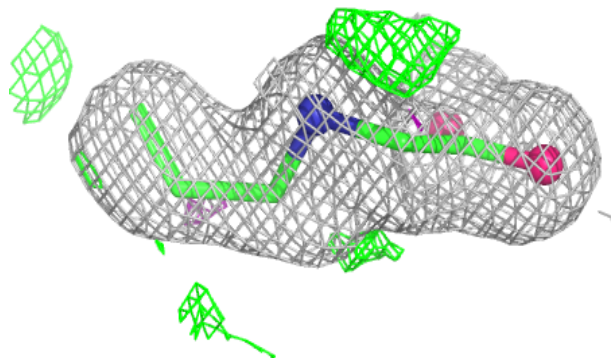
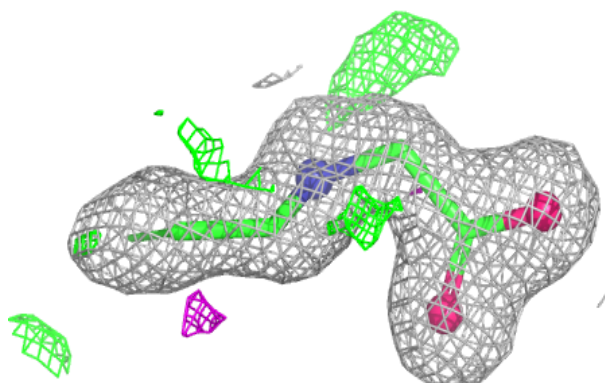


Electron density around CBG B 1302:

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

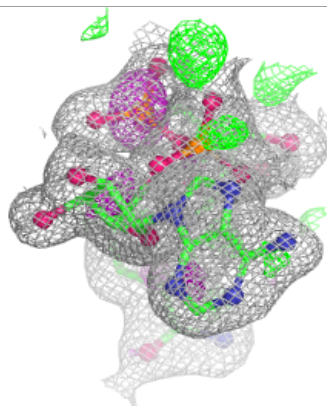
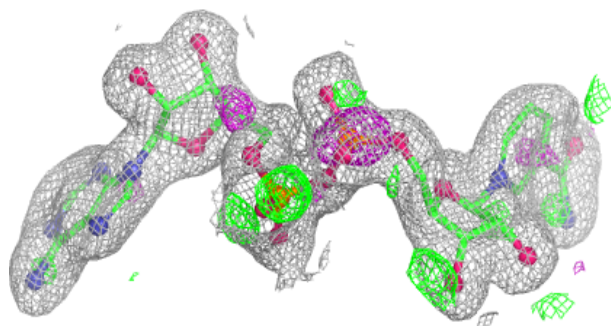
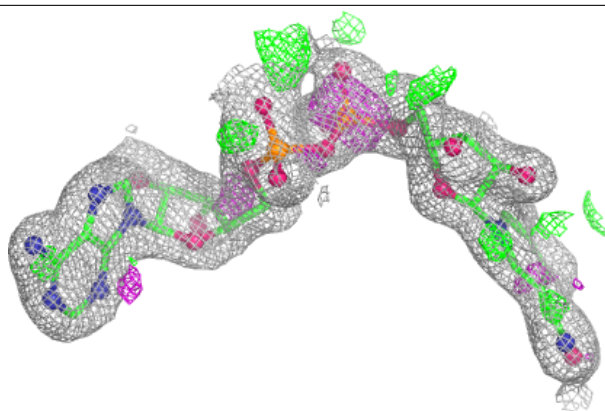
**Electron density around A1AV8 B 1303:**

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

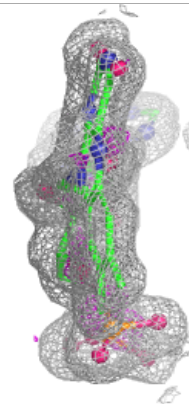
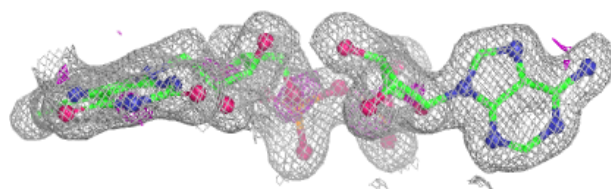
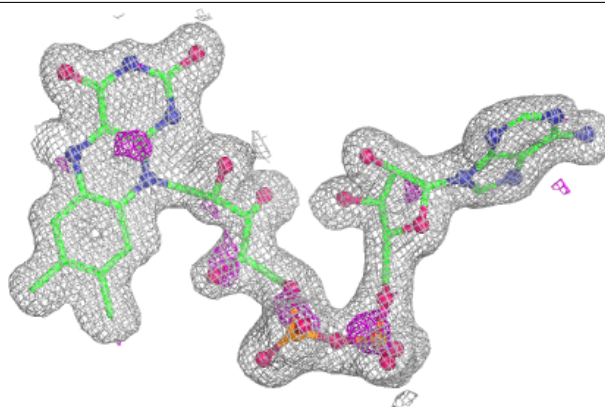


Electron density around NAD A 1303:

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

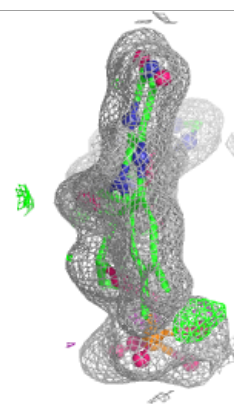
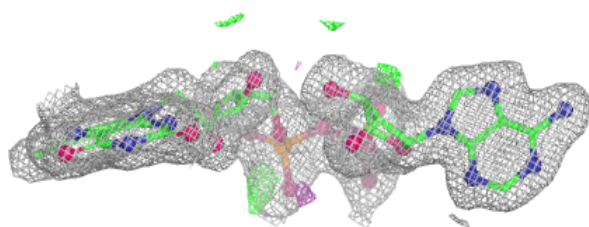
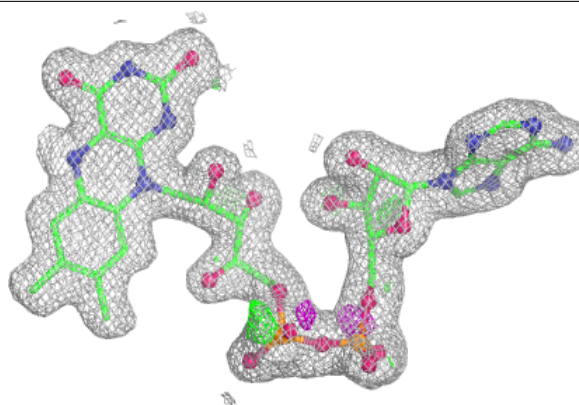
**Electron density around FDA A 1301:**

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

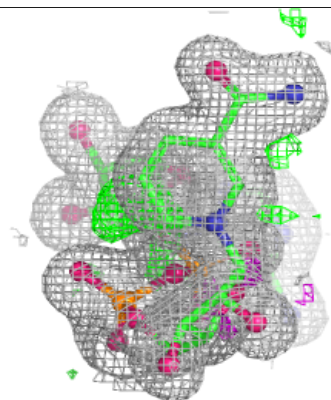
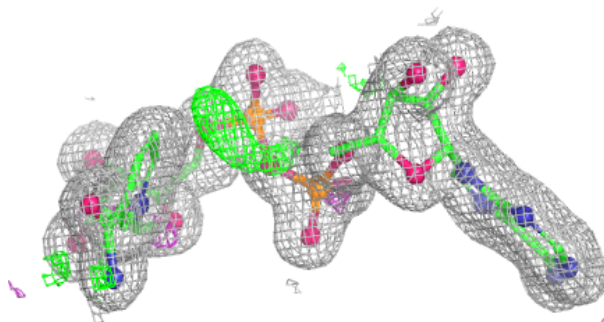
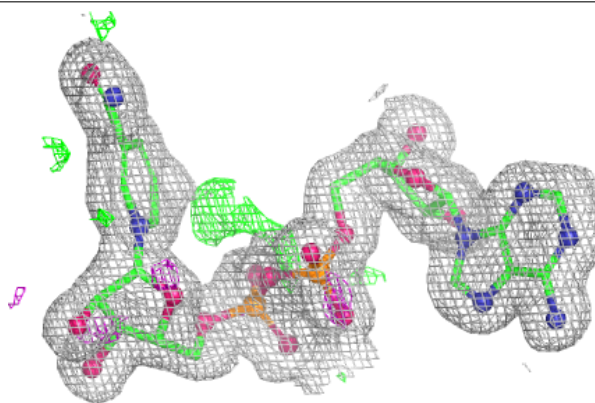


Electron density around FDA B 1301:

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

**Electron density around NAD B 1304:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.