Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 02:38 PM UTC

PDB ID	:	6O4B / pdb_00006o4b
Title	:	Structure of ALDH7A1 mutant W175G complexed with NAD
Authors	:	Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on	:	2019-02-28
Resolution	:	1.85 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 (i) 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 (i)) were used in the production of this report:

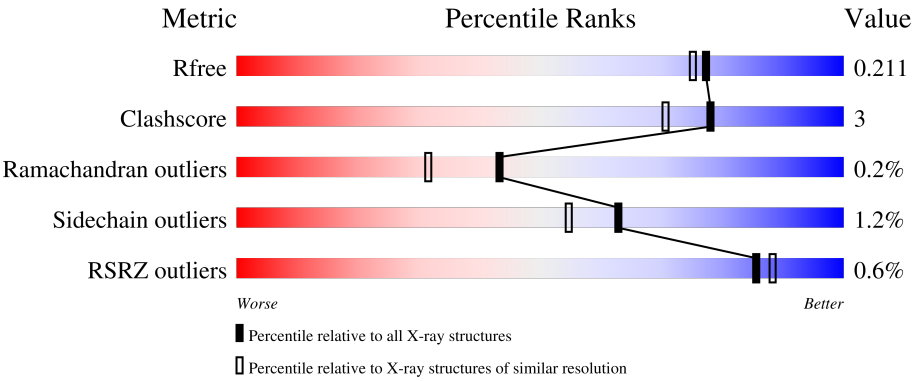
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 <=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	513	92% 8%
1	B	513	90% 9%
1	C	513	91% 8%
1	D	513	93% 6%
1	E	513	93% 6%

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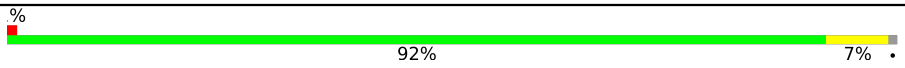
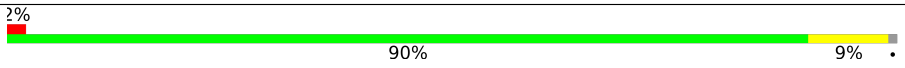
Mol	Chain	Length	Quality of chain
1	F	513	
1	G	513	
1	H	513	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 33057 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	2	0
			3848	2445	665	720	18			
1	B	509	Total	C	N	O	S	0	2	0
			3862	2454	670	720	18			
1	C	509	Total	C	N	O	S	0	1	0
			3852	2445	670	719	18			
1	D	509	Total	C	N	O	S	0	3	0
			3857	2451	668	720	18			
1	E	509	Total	C	N	O	S	0	3	0
			3859	2455	670	717	17			
1	F	509	Total	C	N	O	S	0	1	0
			3873	2457	676	723	17			
1	G	509	Total	C	N	O	S	0	3	0
			3854	2449	665	723	17			
1	H	509	Total	C	N	O	S	0	1	0
			3849	2444	668	719	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	175	GLY	TRP	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	175	GLY	TRP	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	175	GLY	TRP	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	175	GLY	TRP	engineered mutation	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419

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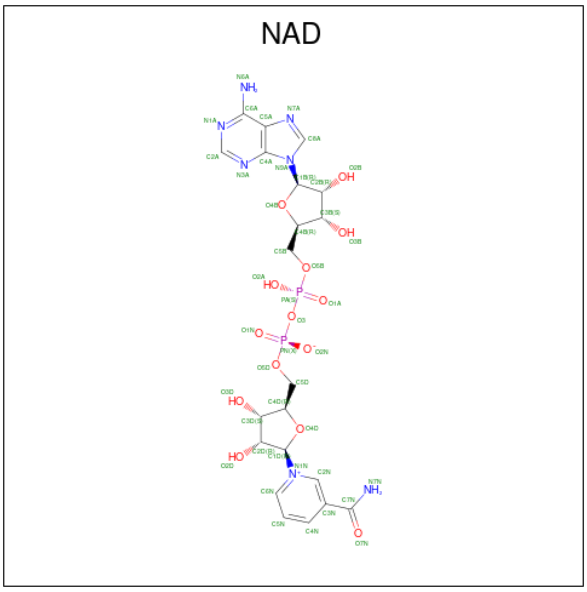
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P49419
E	175	GLY	TRP	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	175	GLY	TRP	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	175	GLY	TRP	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	175	GLY	TRP	engineered mutation	UNP P49419

- 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	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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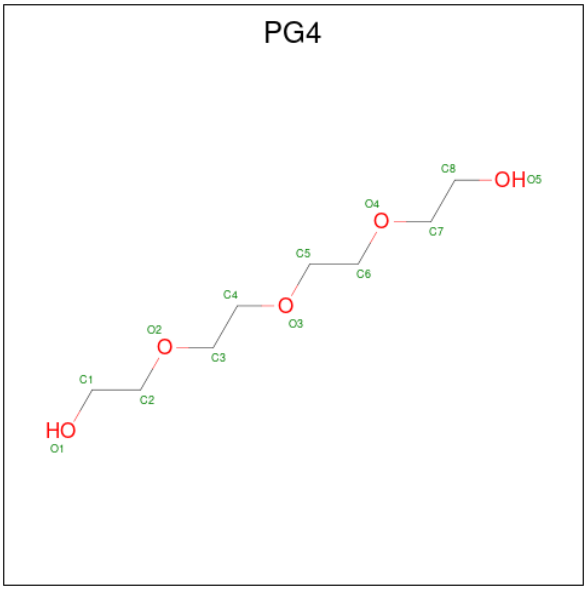
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C N O P 44 21 7 14 2	0	0
2	G	1	Total C N O P 44 21 7 14 2	0	0
2	H	1	Total C N O P 44 21 7 14 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	2	Total Cl 2 2	0	0
3	G	2	Total Cl 2 2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0

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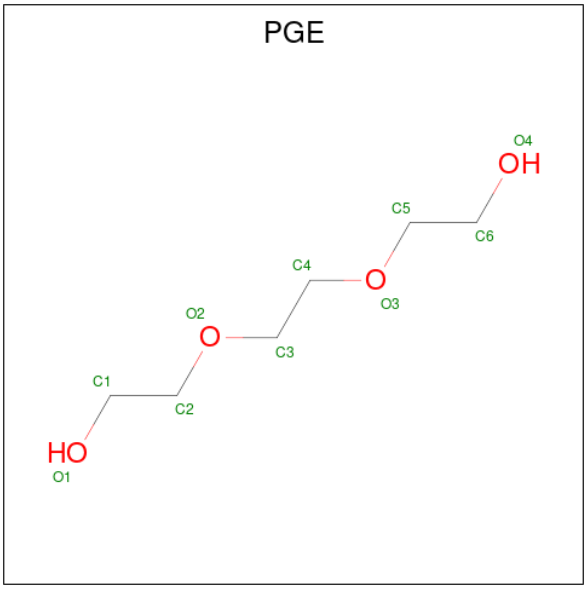
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 8 5	0	0
4	D	1	Total C O 13 8 5	0	0
4	E	1	Total C O 13 8 5	0	0
4	F	1	Total C O 13 8 5	0	0
4	H	1	Total C O 13 8 5	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0

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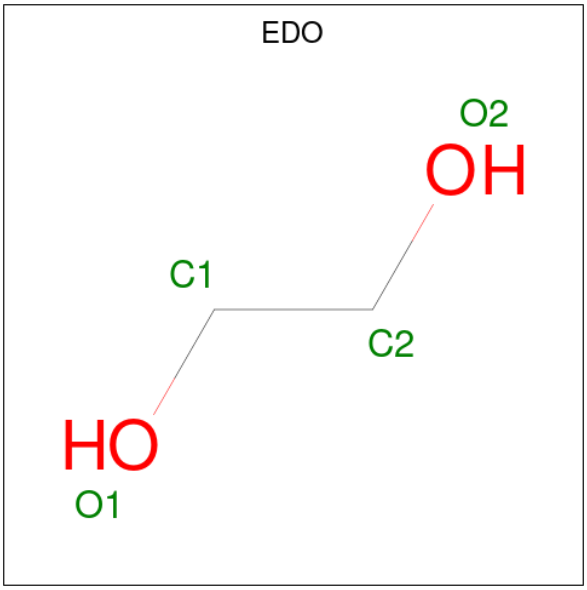
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 10 6 4	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 10 6 4	0	0
5	H	1	Total C O 10 6 4	0	0
5	H	1	Total C O 10 6 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

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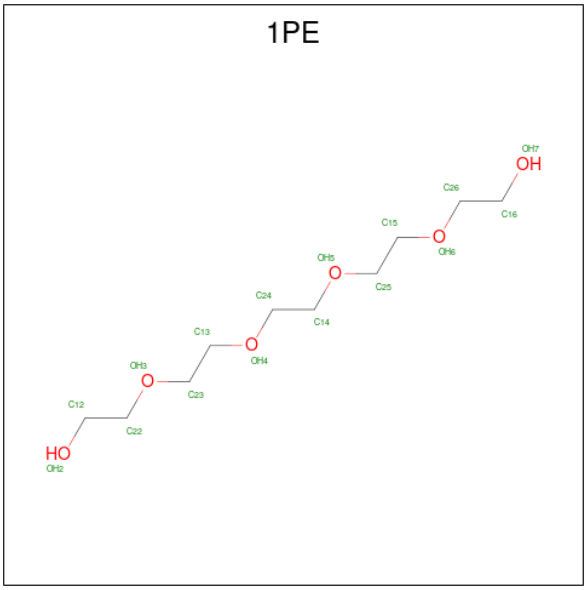
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 16 10 6	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	211	Total O 211 211	0	0
8	B	188	Total O 188 188	0	0
8	C	216	Total O 216 216	0	0
8	D	169	Total O 169 169	0	0
8	E	215	Total O 215 215	0	0
8	F	195	Total O 195 195	0	0

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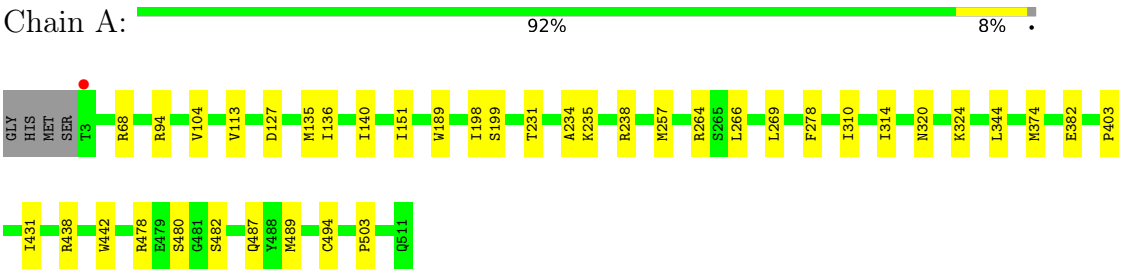
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	189	Total O 189 189	0	0
8	H	208	Total O 209 209	0	1

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.

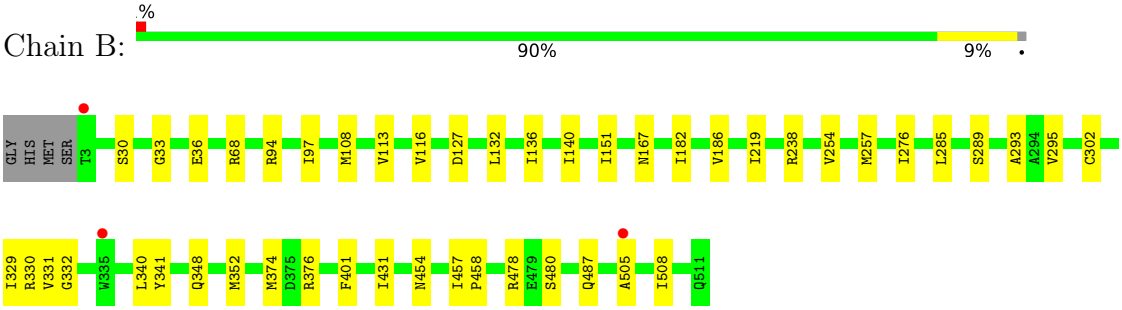
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain A:



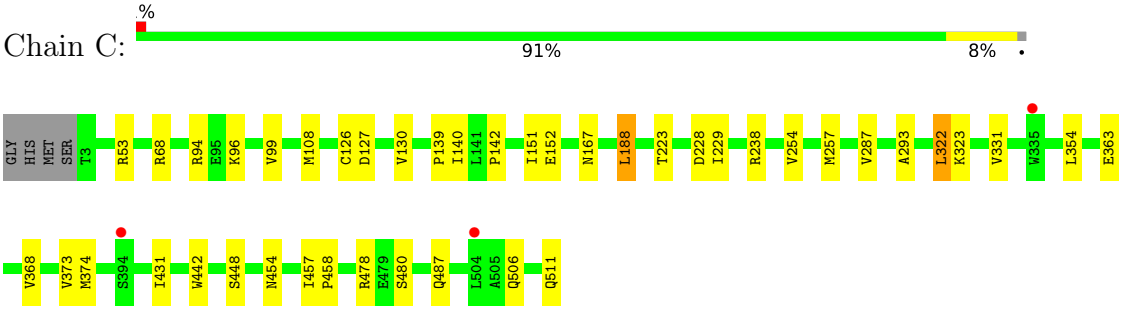
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain B:



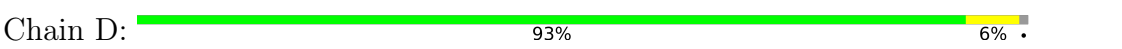
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

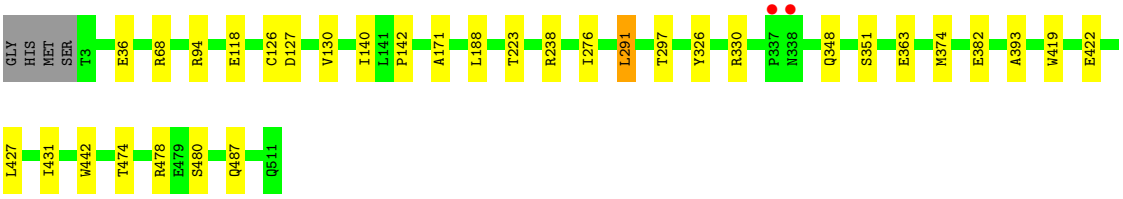
Chain C:



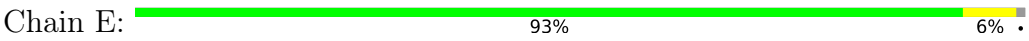
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

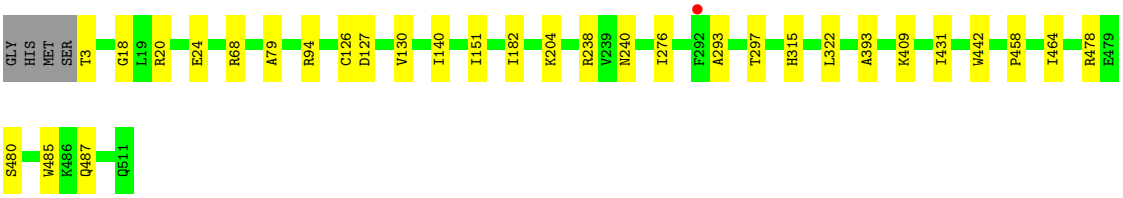
Chain D:



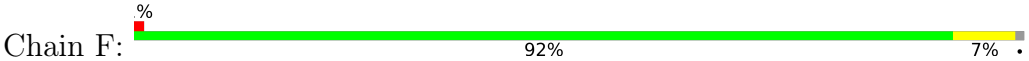


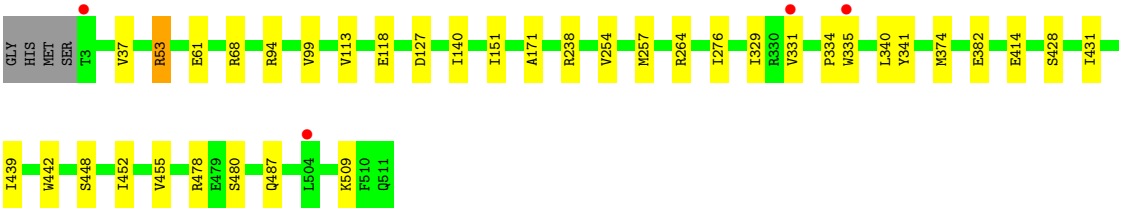
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



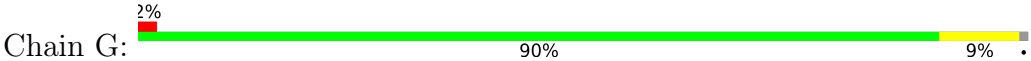


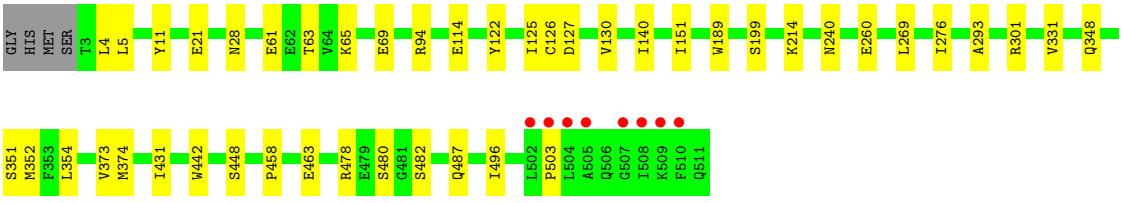
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



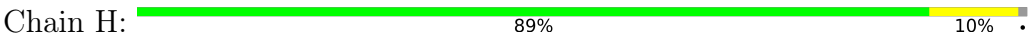


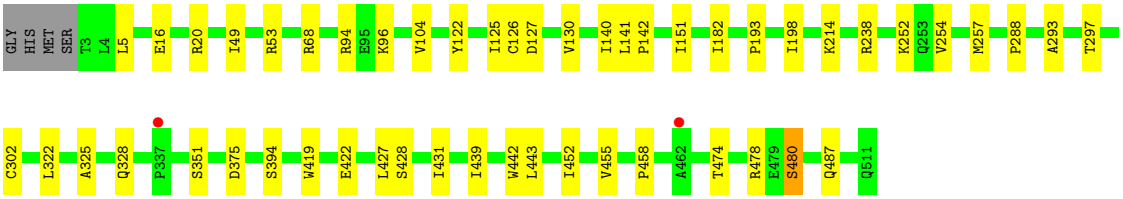
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase





• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.15Å 161.49Å 158.59Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	62.78 – 1.85 62.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	89.6 (62.78-1.85) 94.6 (62.78-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.170 , 0.212 0.168 , 0.211	Depositor DCC
R_{free} test set	15642 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33057	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 1PE, NAD, EDO, CL, PGE

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	0.28	0/3931	0.47	0/5335
1	B	0.25	0/3945	0.45	0/5350
1	C	0.27	0/3932	0.47	0/5334
1	D	0.24	0/3943	0.43	0/5351
1	E	0.27	0/3946	0.46	0/5353
1	F	0.28	0/3953	0.47	0/5358
1	G	0.25	0/3940	0.46	0/5348
1	H	0.26	0/3929	0.45	0/5330
All	All	0.26	0/31519	0.46	0/42759

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

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	3848	0	3831	26	0
1	B	3862	0	3864	27	0
1	C	3852	0	3842	27	0
1	D	3857	0	3849	16	0
1	E	3859	0	3859	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3873	0	3883	22	0
1	G	3854	0	3834	26	0
1	H	3849	0	3836	27	0
2	A	44	0	24	1	0
2	B	44	0	24	1	0
2	C	44	0	25	0	0
2	D	44	0	25	0	0
2	E	44	0	25	0	0
2	F	44	0	24	0	0
2	G	44	0	24	1	0
2	H	44	0	25	1	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	13	0	18	1	0
4	B	13	0	18	0	0
4	D	13	0	18	0	0
4	E	13	0	18	3	0
4	F	13	0	18	0	0
4	H	13	0	18	1	0
5	A	20	0	28	2	0
5	B	10	0	14	0	0
5	C	10	0	14	0	0
5	D	10	0	14	0	0
5	E	20	0	28	1	0
5	F	20	0	28	2	0
5	G	27	0	37	3	0
5	H	20	0	28	1	0
6	A	4	0	6	0	0
6	C	4	0	6	0	0
6	D	8	0	12	0	0
6	E	4	0	6	0	0
7	C	16	0	22	0	0
8	A	211	0	0	2	0
8	B	188	0	0	0	0
8	C	216	0	0	2	0
8	D	169	0	0	0	0
8	E	215	0	0	1	0
8	F	195	0	0	3	0
8	G	189	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	209	0	0	1	0
All	All	33057	0	31345	175	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 3.

All (175) 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:348:GLN:HG2	1:B:352:MET:HE2	1.65	0.79
1:F:140:ILE:HD11	1:G:151:ILE:HB	1.67	0.76
1:E:151:ILE:HB	1:H:140:ILE:HD11	1.68	0.75
1:A:235:LYS:HG3	1:A:257:MET:HE3	1.70	0.74
1:C:323:LYS:HE2	1:C:368:VAL:HB	1.68	0.74
1:B:151:ILE:HB	1:C:140:ILE:HD11	1.70	0.73
1:C:478:ARG:O	1:C:487:GLN:NE2	2.23	0.70
1:G:478:ARG:O	1:G:487:GLN:NE2	2.21	0.70
1:F:478:ARG:O	1:F:487:GLN:NE2	2.24	0.70
1:B:140:ILE:HD11	1:C:151:ILE:HB	1.79	0.65
1:F:151:ILE:HB	1:G:140:ILE:HD11	1.78	0.65
1:A:478:ARG:O	1:A:487:GLN:NE2	2.29	0.65
1:E:478:ARG:O	1:E:487:GLN:NE2	2.29	0.64
1:A:482:SER:HA	5:A:606:PGE:H5	1.80	0.63
1:H:16:GLU:O	1:H:96:LYS:NZ	2.31	0.63
1:A:151:ILE:HB	1:D:140:ILE:HD11	1.81	0.62
1:H:94:ARG:NH2	1:H:127:ASP:OD2	2.30	0.61
1:A:231:THR:HG23	1:A:257:MET:HE1	1.82	0.61
1:H:325:ALA:HA	1:H:328:GLN:HE21	1.64	0.60
1:F:94:ARG:NH2	1:F:127:ASP:OD2	2.35	0.60
1:D:118:GLU:HG3	1:D:171:ALA:HB2	1.85	0.57
1:G:354:LEU:HD21	1:G:373:VAL:HG23	1.85	0.57
1:B:140:ILE:HG13	1:C:140:ILE:HG13	1.86	0.56
1:E:3:THR:N	8:E:701:HOH:O	2.38	0.56
1:H:478:ARG:O	1:H:487:GLN:NE2	2.37	0.56
1:B:331:VAL:HG21	1:B:374:MET:HE1	1.87	0.55
1:E:94:ARG:NH2	1:E:127:ASP:OD2	2.37	0.55
1:E:68:ARG:HH21	4:E:604:PG4:H22	1.71	0.55
1:C:331:VAL:HG21	1:C:374:MET:HE1	1.89	0.55
1:F:37:VAL:HG22	1:F:53:ARG:HD3	1.88	0.55
1:A:264:ARG:NH1	1:A:489:MET:O	2.35	0.54
1:H:293:ALA:HB2	1:H:458:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:VAL:HG13	1:F:341:TYR:HD2	1.73	0.54
1:G:496:ILE:HD11	1:H:443:LEU:HD11	1.89	0.54
1:C:506:GLN:O	1:D:330:ARG:NH1	2.40	0.54
1:A:136:ILE:O	1:D:142:PRO:HD3	2.08	0.54
1:G:293:ALA:HB2	1:G:458:PRO:HB2	1.89	0.53
1:D:94:ARG:NH2	1:D:127:ASP:OD2	2.38	0.53
1:G:65:LYS:O	1:G:69:GLU:HG2	2.08	0.53
1:E:68:ARG:HD2	1:E:238:ARG:HB3	1.91	0.53
1:A:310:ILE:HG22	1:A:314:ILE:HG13	1.91	0.52
1:C:68:ARG:HD2	1:C:238:ARG:HB3	1.91	0.52
1:B:478:ARG:O	1:B:487:GLN:NE2	2.38	0.52
1:F:264[B]:ARG:NH2	8:F:705:HOH:O	2.43	0.52
1:E:126:CYS:O	1:E:130:VAL:HG23	2.10	0.51
1:C:354:LEU:HD21	1:C:373:VAL:HG23	1.91	0.51
1:G:94:ARG:NH2	1:G:127:ASP:OD2	2.40	0.51
1:B:331:VAL:HG13	1:B:341:TYR:HD2	1.75	0.51
1:B:329:ILE:HG23	1:B:340:LEU:HD23	1.93	0.51
1:B:94:ARG:NH2	1:B:127:ASP:OD2	2.34	0.51
1:B:332:GLY:HA2	1:B:376:ARG:NH2	2.25	0.51
1:B:97:ILE:HG12	1:B:116:VAL:HG13	1.92	0.50
1:C:287:VAL:HG13	1:C:322:LEU:HD13	1.93	0.50
1:A:151:ILE:HG12	1:A:494:CYS:HB2	1.94	0.50
1:H:104:VAL:HA	1:H:198:ILE:HD11	1.94	0.50
1:G:331:VAL:HG21	1:G:374:MET:HE1	1.92	0.50
1:B:289:SER:HB3	1:B:458:PRO:HD3	1.94	0.50
1:E:18:GLY:O	1:E:204:LYS:NZ	2.38	0.49
1:A:264:ARG:NH2	8:A:702:HOH:O	2.39	0.49
1:G:114:GLU:OE2	1:G:301:ARG:NH1	2.42	0.49
1:A:234:ALA:HB3	1:A:257:MET:HE2	1.95	0.49
1:A:431:ILE:HG23	1:A:442:TRP:CE2	2.48	0.49
1:B:151:ILE:HB	1:C:140:ILE:CD1	2.42	0.49
1:E:293:ALA:HB2	1:E:458:PRO:HB2	1.95	0.49
1:H:68:ARG:NH2	4:H:602:PG4:H61	2.28	0.49
1:B:36:GLU:OE2	1:E:393:ALA:HA	2.14	0.48
1:F:374:MET:HE3	1:F:382:GLU:HA	1.96	0.48
1:A:135:MET:HB3	5:A:606:PGE:H2	1.95	0.48
1:G:4:LEU:HD12	1:G:21:GLU:HG2	1.94	0.48
1:D:478:ARG:O	1:D:487:GLN:NE2	2.43	0.48
1:C:94:ARG:NH2	1:C:127:ASP:OD2	2.40	0.48
1:H:122:TYR:HA	1:H:125:ILE:HG22	1.95	0.48
1:F:254:VAL:HA	1:F:257:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:NH2	1:A:127:ASP:OD2	2.41	0.47
1:C:126:CYS:O	1:C:130:VAL:HG23	2.15	0.47
1:F:118:GLU:HG3	1:F:171:ALA:HB2	1.95	0.47
1:A:278:PHE:CZ	1:A:438:ARG:HD3	2.50	0.47
1:A:235:LYS:HG3	1:A:257:MET:CE	2.43	0.47
1:A:269:LEU:O	2:A:601:NAD:H2N	2.15	0.47
1:C:431:ILE:HG23	1:C:442:TRP:CE2	2.49	0.47
1:F:113:VAL:HG13	8:F:868:HOH:O	2.15	0.47
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.96	0.47
1:F:329:ILE:HG23	1:F:340:LEU:HD23	1.97	0.47
1:B:108:MET:HE3	1:B:167:ASN:HA	1.97	0.46
1:C:442:TRP:CH2	1:C:448:SER:HB2	2.51	0.46
1:E:240:ASN:HD21	4:E:604:PG4:H71	1.80	0.46
1:G:28:ASN:HB3	1:G:63:THR:HG23	1.98	0.46
1:C:96:LYS:NZ	8:C:710:HOH:O	2.49	0.46
1:C:108:MET:HE3	1:C:167:ASN:HA	1.98	0.45
1:E:431:ILE:HG23	1:E:442:TRP:CE2	2.51	0.45
1:H:480:SER:HB2	5:H:603:PGE:H22	1.99	0.45
1:A:344:LEU:HD21	1:A:403:PRO:HD3	1.98	0.45
1:D:419:TRP:O	1:D:422:GLU:HG2	2.17	0.45
1:B:293:ALA:HB2	1:B:458:PRO:HB2	1.99	0.45
1:D:374:MET:HE3	1:D:382:GLU:HA	1.99	0.45
1:G:240:ASN:HD21	5:G:605:PGE:H12	1.82	0.45
1:G:442:TRP:CH2	1:G:448:SER:HB2	2.51	0.45
1:B:140:ILE:CD1	1:C:151:ILE:HB	2.44	0.45
1:E:20:ARG:HH22	1:E:24:GLU:CD	2.25	0.44
1:E:68:ARG:NH2	4:E:604:PG4:H22	2.32	0.44
1:E:140:ILE:HD11	1:H:151:ILE:HB	1.99	0.44
1:F:331:VAL:HG21	1:F:374:MET:HE1	1.99	0.44
1:G:126:CYS:O	1:G:130:VAL:HG23	2.17	0.44
1:B:454:ASN:HB3	1:B:457:ILE:HG23	2.00	0.44
1:H:427:LEU:HD13	1:H:474:THR:HG21	2.00	0.44
1:E:315:HIS:CD2	1:E:409:LYS:HG2	2.52	0.44
1:H:439:ILE:HG23	1:H:455:VAL:HG21	1.98	0.44
1:E:276:ILE:HB	1:E:431:ILE:HG22	1.98	0.44
1:D:126:CYS:O	1:D:130:VAL:HG23	2.18	0.44
1:E:464:ILE:HG23	8:F:816:HOH:O	2.17	0.44
1:F:140:ILE:HG13	1:G:140:ILE:HG13	2.00	0.44
1:F:431:ILE:HG23	1:F:442:TRP:CE2	2.52	0.44
1:H:254:VAL:HA	1:H:257:MET:HE3	2.00	0.44
1:F:61:GLU:OE2	1:F:238:ARG:NH2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:ILE:HG23	1:F:455:VAL:HG21	2.00	0.44
1:A:503:PRO:HD3	1:B:285:LEU:HD12	2.00	0.43
1:H:193:PRO:HD2	8:H:793:HOH:O	2.18	0.43
1:B:276:ILE:HB	1:B:431:ILE:HG22	1.99	0.43
1:D:291:LEU:HD12	1:D:326:TYR:CD1	2.53	0.43
1:H:126:CYS:O	1:H:130:VAL:HG23	2.19	0.43
1:H:428:SER:HA	1:H:452:ILE:HB	1.99	0.43
1:D:68:ARG:HD2	1:D:238:ARG:HB3	2.01	0.43
1:H:68:ARG:HD2	1:H:238:ARG:HB3	2.00	0.43
1:G:260:GLU:O	1:H:252:LYS:HE3	2.19	0.43
1:C:254:VAL:HA	1:C:257:MET:HE3	2.01	0.43
1:D:427:LEU:HD13	1:D:474:THR:HG21	2.01	0.43
1:G:61:GLU:O	1:G:65:LYS:HG3	2.18	0.43
1:H:419:TRP:O	1:H:422:GLU:HG2	2.19	0.43
1:B:68:ARG:HD2	1:B:238:ARG:HB3	2.01	0.42
1:G:503:PRO:HG2	1:H:288:PRO:HB2	2.01	0.42
1:A:320:ASN:O	1:A:324:LYS:HG3	2.20	0.42
1:C:99:VAL:HG22	8:C:887:HOH:O	2.19	0.42
5:F:603:PGE:H2	5:F:603:PGE:H52	2.01	0.42
1:G:276:ILE:HB	1:G:431:ILE:HG22	2.01	0.42
1:H:431:ILE:HG23	1:H:442:TRP:CE2	2.54	0.42
1:B:136:ILE:O	1:C:142:PRO:HD3	2.20	0.42
1:A:235:LYS:HE3	1:A:257:MET:HE3	2.01	0.42
1:B:505:ALA:HB1	1:B:508:ILE:O	2.19	0.42
1:G:122:TYR:O	1:G:125[B]:ILE:HG22	2.19	0.42
1:G:189:TRP:CH2	1:G:199:SER:HA	2.54	0.42
1:A:113:VAL:HG13	8:A:811:HOH:O	2.19	0.42
1:F:442:TRP:CH2	1:F:448:SER:HB2	2.55	0.42
1:F:276:ILE:HB	1:F:431:ILE:HG22	2.02	0.42
1:D:276:ILE:HB	1:D:431:ILE:HG22	2.02	0.42
1:A:104:VAL:HA	1:A:198:ILE:HD11	2.01	0.42
1:D:431:ILE:HG23	1:D:442:TRP:CE2	2.55	0.42
1:G:5:LEU:HD22	1:G:11:TYR:CE2	2.55	0.42
1:G:269:LEU:O	2:G:601:NAD:H2N	2.20	0.42
5:G:606:PGE:H6	1:H:141:LEU:HD21	2.02	0.42
1:B:186:VAL:HG12	1:B:219:ILE:HA	2.01	0.41
4:A:604:PG4:H52	4:A:604:PG4:H32	1.81	0.41
1:B:132[B]:LEU:HD23	1:B:132[B]:LEU:HA	1.90	0.41
1:H:5:LEU:HB2	1:H:49:ILE:HA	2.02	0.41
1:A:374:MET:HE3	1:A:382:GLU:HA	2.02	0.41
1:D:188:LEU:HD11	1:D:223:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:482:SER:HA	5:G:606:PGE:H52	2.03	0.41
1:B:254:VAL:HA	1:B:257:MET:HE3	2.03	0.41
1:E:485:TRP:HE1	5:E:606:PGE:C6	2.34	0.41
5:F:604:PGE:H22	5:F:604:PGE:H4	1.98	0.41
1:C:139:PRO:HD2	1:C:152:GLU:HB3	2.02	0.41
1:E:79:ALA:HB3	1:H:142:PRO:HB2	2.03	0.41
1:F:68:ARG:HD2	1:F:238:ARG:HB3	2.03	0.41
1:G:431:ILE:HG23	1:G:442:TRP:CE2	2.56	0.41
1:A:189:TRP:CH2	1:A:199:SER:HA	2.56	0.40
1:C:188:LEU:HD21	1:C:223:THR:HG23	2.03	0.40
1:F:428:SER:HA	1:F:452:ILE:HB	2.02	0.40
1:H:302:CYS:HB3	2:H:601:NAD:C2N	2.52	0.40
1:B:302:CYS:HB3	2:B:601:NAD:C2N	2.51	0.40
1:C:478:ARG:C	1:C:487:GLN:HE22	2.23	0.40
1:E:322[B]:LEU:HD23	1:E:322[B]:LEU:HA	1.93	0.40
1:F:334:PRO:HD2	1:F:335:TRP:CZ3	2.57	0.40
1:C:228:ASP:OD1	1:C:229:ILE:N	2.53	0.40
1:C:293:ALA:HB2	1:C:458:PRO:HB2	2.04	0.40
1:C:454:ASN:HB3	1:C:457:ILE:HG23	2.02	0.40
1:D:363:GLU:OE1	1:D:393:ALA:HB1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/513 (99%)	494 (97%)	14 (3%)	1 (0%)	43	31
1	B	509/513 (99%)	494 (97%)	13 (3%)	2 (0%)	30	17
1	C	508/513 (99%)	490 (96%)	17 (3%)	1 (0%)	43	31
1	D	510/513 (99%)	492 (96%)	17 (3%)	1 (0%)	43	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	510/513 (99%)	492 (96%)	17 (3%)	1 (0%)	43 31
1	F	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	43 31
1	G	510/513 (99%)	496 (97%)	13 (2%)	1 (0%)	43 31
1	H	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	43 31
All	All	4072/4104 (99%)	3942 (97%)	121 (3%)	9 (0%)	43 31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	B	480	SER
1	C	480	SER
1	D	480	SER
1	F	480	SER
1	H	480	SER
1	E	480	SER
1	G	480	SER
1	B	33	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	399/409 (98%)	397 (100%)	2 (0%)	81 77
1	B	402/409 (98%)	396 (98%)	6 (2%)	57 47
1	C	400/409 (98%)	395 (99%)	5 (1%)	61 51
1	D	401/409 (98%)	396 (99%)	5 (1%)	63 55
1	E	401/409 (98%)	399 (100%)	2 (0%)	81 77
1	F	405/409 (99%)	401 (99%)	4 (1%)	68 60
1	G	400/409 (98%)	395 (99%)	5 (1%)	61 51
1	H	399/409 (98%)	390 (98%)	9 (2%)	44 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3207/3272 (98%)	3169 (99%)	38 (1%)	63 55

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ILE
1	A	266	LEU
1	B	30	SER
1	B	113	VAL
1	B	182	ILE
1	B	295	VAL
1	B	330	ARG
1	B	401	PHE
1	C	53	ARG
1	C	188	LEU
1	C	322	LEU
1	C	363	GLU
1	C	511	GLN
1	D	36	GLU
1	D	291	LEU
1	D	297	THR
1	D	348	GLN
1	D	351	SER
1	E	182	ILE
1	E	297	THR
1	F	53	ARG
1	F	99	VAL
1	F	414	GLU
1	F	509	LYS
1	G	214	LYS
1	G	348	GLN
1	G	351	SER
1	G	352	MET
1	G	463	GLU
1	H	20	ARG
1	H	53	ARG
1	H	182	ILE
1	H	214	LYS
1	H	297	THR
1	H	322	LEU
1	H	351	SER
1	H	375	ASP

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Mol	Chain	Res	Type
1	H	394	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	153	GLN
1	A	155	ASN
1	A	177	ASN
1	A	213	ASN
1	B	46	ASN
1	B	153	GLN
1	B	155	ASN
1	B	177	ASN
1	B	253	GLN
1	B	338	ASN
1	B	379	ASN
1	C	120	GLN
1	C	153	GLN
1	C	155	ASN
1	C	177	ASN
1	C	333	ASN
1	C	348	GLN
1	C	412	ASN
1	D	46	ASN
1	D	88	GLN
1	D	155	ASN
1	D	213	ASN
1	D	379	ASN
1	E	98	GLN
1	E	155	ASN
1	E	249	GLN
1	F	10	GLN
1	F	155	ASN
1	F	177	ASN
1	F	213	ASN
1	G	46	ASN
1	G	54	GLN
1	G	155	ASN
1	G	177	ASN
1	G	213	ASN
1	G	259	GLN

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Mol	Chain	Res	Type
1	G	338	ASN
1	G	348	GLN
1	G	379	ASN
1	H	153	GLN
1	H	155	ASN
1	H	177	ASN
1	H	328	GLN
1	H	379	ASN

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 42 ligands modelled in this entry, 8 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
2	NAD	H	601	-	46,48,48	3.55	13 (28%)	64,73,73	1.65	11 (17%)
2	NAD	A	601	-	46,48,48	3.54	16 (34%)	64,73,73	1.68	13 (20%)
4	PG4	D	603	-	12,12,12	0.68	0	11,11,11	0.27	0
5	PGE	H	603	-	9,9,9	0.50	0	8,8,8	0.29	0
5	PGE	F	603	-	9,9,9	0.51	0	8,8,8	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	C	604	-	3,3,3	0.45	0	2,2,2	0.26	0
5	PGE	C	603	-	9,9,9	0.56	0	8,8,8	0.31	0
2	NAD	G	601	-	46,48,48	3.58	14 (30%)	64,73,73	1.63	11 (17%)
5	PGE	H	604	-	9,9,9	0.55	0	8,8,8	0.24	0
5	PGE	A	605	-	9,9,9	0.55	0	8,8,8	0.22	0
4	PG4	B	602	-	12,12,12	0.62	0	11,11,11	0.28	0
5	PGE	D	604	-	9,9,9	0.58	0	8,8,8	0.30	0
2	NAD	B	601	-	46,48,48	3.57	16 (34%)	64,73,73	1.70	11 (17%)
4	PG4	E	604	-	12,12,12	0.71	0	11,11,11	0.40	0
7	1PE	C	605	-	15,15,15	0.53	0	14,14,14	0.34	0
4	PG4	F	602	-	12,12,12	0.65	0	11,11,11	0.31	0
5	PGE	G	605	-	6,6,9	0.56	0	5,5,8	0.26	0
2	NAD	E	601	-	46,48,48	3.56	17 (36%)	64,73,73	1.69	14 (21%)
4	PG4	A	604	-	12,12,12	0.64	0	11,11,11	0.35	0
6	EDO	D	605	-	3,3,3	0.44	0	2,2,2	0.42	0
2	NAD	F	601	-	46,48,48	3.57	17 (36%)	64,73,73	1.70	11 (17%)
6	EDO	A	607	-	3,3,3	0.45	0	2,2,2	0.28	0
5	PGE	B	603	-	9,9,9	0.52	0	8,8,8	0.31	0
5	PGE	E	605	-	9,9,9	0.55	0	8,8,8	0.31	0
5	PGE	E	606	-	9,9,9	0.56	0	8,8,8	0.26	0
5	PGE	F	604	-	9,9,9	0.53	0	8,8,8	0.26	0
2	NAD	D	601	-	46,48,48	3.58	16 (34%)	64,73,73	1.62	11 (17%)
2	NAD	C	601	-	46,48,48	3.58	15 (32%)	64,73,73	1.70	14 (21%)
5	PGE	G	604	-	9,9,9	0.53	0	8,8,8	0.40	0
4	PG4	H	602	-	12,12,12	0.64	0	11,11,11	0.23	0
5	PGE	G	606	-	9,9,9	0.53	0	8,8,8	0.39	0
5	PGE	A	606	-	9,9,9	0.47	0	8,8,8	0.31	0
6	EDO	D	606	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	E	607	-	3,3,3	0.49	0	2,2,2	0.50	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
2	NAD	H	601	-	-	5/30/62/62	0/5/5/5
2	NAD	A	601	-	-	5/30/62/62	0/5/5/5
4	PG4	D	603	-	-	5/10/10/10	-
5	PGE	H	603	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	F	603	-	-	5/7/7/7	-
6	EDO	C	604	-	-	1/1/1/1	-
5	PGE	C	603	-	-	2/7/7/7	-
2	NAD	G	601	-	-	5/30/62/62	0/5/5/5
5	PGE	H	604	-	-	0/7/7/7	-
5	PGE	A	605	-	-	1/7/7/7	-
4	PG4	B	602	-	-	1/10/10/10	-
5	PGE	D	604	-	-	4/7/7/7	-
2	NAD	B	601	-	-	4/30/62/62	0/5/5/5
4	PG4	E	604	-	-	6/10/10/10	-
7	1PE	C	605	-	-	4/13/13/13	-
4	PG4	F	602	-	-	2/10/10/10	-
5	PGE	G	605	-	-	2/4/4/7	-
2	NAD	E	601	-	-	6/30/62/62	0/5/5/5
4	PG4	A	604	-	-	6/10/10/10	-
6	EDO	D	605	-	-	0/1/1/1	-
2	NAD	F	601	-	-	5/30/62/62	0/5/5/5
6	EDO	A	607	-	-	1/1/1/1	-
5	PGE	B	603	-	-	4/7/7/7	-
5	PGE	E	605	-	-	5/7/7/7	-
5	PGE	E	606	-	-	4/7/7/7	-
5	PGE	F	604	-	-	5/7/7/7	-
2	NAD	D	601	-	-	4/30/62/62	0/5/5/5
2	NAD	C	601	-	-	4/30/62/62	0/5/5/5
5	PGE	G	604	-	-	4/7/7/7	-
4	PG4	H	602	-	-	5/10/10/10	-
5	PGE	G	606	-	-	2/7/7/7	-
5	PGE	A	606	-	-	7/7/7/7	-
6	EDO	D	606	-	-	0/1/1/1	-
6	EDO	E	607	-	-	1/1/1/1	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NAD	O4D-C1D	15.83	1.61	1.40
2	A	601	NAD	O4D-C1D	15.77	1.61	1.40
2	F	601	NAD	O4D-C1D	15.58	1.61	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	O4D-C1D	15.58	1.61	1.40
2	D	601	NAD	O4D-C1D	15.55	1.61	1.40
2	B	601	NAD	O4D-C1D	15.50	1.61	1.40
2	H	601	NAD	O4D-C1D	15.50	1.61	1.40
2	G	601	NAD	O4D-C1D	15.41	1.61	1.40
2	B	601	NAD	O4B-C1B	8.83	1.62	1.42
2	G	601	NAD	O4B-C1B	8.57	1.61	1.42
2	D	601	NAD	O4B-C1B	8.31	1.61	1.42
2	C	601	NAD	O4B-C1B	8.19	1.60	1.42
2	H	601	NAD	O4B-C1B	8.11	1.60	1.42
2	E	601	NAD	O4B-C1B	8.09	1.60	1.42
2	F	601	NAD	O4B-C1B	7.88	1.60	1.42
2	A	601	NAD	O4B-C1B	7.68	1.59	1.42
2	C	601	NAD	C2B-C1B	-7.63	1.29	1.53
2	H	601	NAD	C2B-C1B	-7.60	1.29	1.53
2	G	601	NAD	C2B-C1B	-7.50	1.29	1.53
2	D	601	NAD	C2B-C1B	-7.49	1.30	1.53
2	A	601	NAD	C2B-C1B	-7.38	1.30	1.53
2	F	601	NAD	C7N-N7N	7.35	1.46	1.33
2	E	601	NAD	C2B-C1B	-7.25	1.30	1.53
2	B	601	NAD	C2B-C1B	-7.14	1.31	1.53
2	C	601	NAD	C7N-N7N	7.04	1.45	1.33
2	F	601	NAD	C2B-C1B	-7.02	1.31	1.53
2	G	601	NAD	C7N-N7N	6.93	1.45	1.33
2	B	601	NAD	C7N-N7N	6.88	1.45	1.33
2	E	601	NAD	C7N-N7N	6.86	1.45	1.33
2	H	601	NAD	C7N-N7N	6.82	1.45	1.33
2	D	601	NAD	C7N-N7N	6.71	1.45	1.33
2	C	601	NAD	O4B-C4B	-6.31	1.31	1.45
2	A	601	NAD	C7N-N7N	6.28	1.44	1.33
2	H	601	NAD	O4B-C4B	-6.27	1.31	1.45
2	F	601	NAD	O4B-C4B	-6.15	1.31	1.45
2	D	601	NAD	O4B-C4B	-6.12	1.31	1.45
2	G	601	NAD	O4B-C4B	-5.96	1.31	1.45
2	C	601	NAD	O4D-C4D	-5.92	1.31	1.45
2	E	601	NAD	O4B-C4B	-5.80	1.32	1.45
2	D	601	NAD	O4D-C4D	-5.79	1.32	1.45
2	A	601	NAD	O4B-C4B	-5.76	1.32	1.45
2	B	601	NAD	O4D-C4D	-5.76	1.32	1.45
2	B	601	NAD	O4B-C4B	-5.70	1.32	1.45
2	G	601	NAD	O4D-C4D	-5.69	1.32	1.45
2	E	601	NAD	O4D-C4D	-5.61	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	NAD	O4D-C4D	-5.55	1.32	1.45
2	A	601	NAD	O4D-C4D	-5.50	1.32	1.45
2	F	601	NAD	O4D-C4D	-5.45	1.32	1.45
2	A	601	NAD	C2N-N1N	4.12	1.39	1.35
2	D	601	NAD	C6A-N6A	3.94	1.44	1.34
2	A	601	NAD	C6A-N6A	3.84	1.44	1.34
2	D	601	NAD	C3N-C7N	3.78	1.56	1.50
2	C	601	NAD	C6A-N6A	3.75	1.43	1.34
2	F	601	NAD	C6A-N6A	3.67	1.43	1.34
2	B	601	NAD	C6A-N6A	3.63	1.43	1.34
2	G	601	NAD	C6A-N6A	3.51	1.43	1.34
2	H	601	NAD	C6A-N6A	3.51	1.43	1.34
2	E	601	NAD	C2N-N1N	3.51	1.38	1.35
2	F	601	NAD	C3N-C7N	3.49	1.55	1.50
2	E	601	NAD	C6A-N6A	3.46	1.43	1.34
2	D	601	NAD	C2N-N1N	3.43	1.38	1.35
2	A	601	NAD	C3N-C7N	3.39	1.55	1.50
2	F	601	NAD	C2N-N1N	3.38	1.38	1.35
2	G	601	NAD	C3N-C7N	3.35	1.55	1.50
2	B	601	NAD	C2N-N1N	3.35	1.38	1.35
2	G	601	NAD	C2N-N1N	3.24	1.38	1.35
2	H	601	NAD	C3N-C7N	3.22	1.55	1.50
2	C	601	NAD	C3N-C7N	3.19	1.55	1.50
2	E	601	NAD	C3N-C7N	3.16	1.55	1.50
2	B	601	NAD	O3D-C3D	-3.09	1.35	1.43
2	G	601	NAD	O3D-C3D	-3.04	1.35	1.43
2	C	601	NAD	O3D-C3D	-3.03	1.35	1.43
2	A	601	NAD	O3D-C3D	-2.99	1.35	1.43
2	H	601	NAD	O3D-C3D	-2.96	1.35	1.43
2	G	601	NAD	O2B-C2B	2.94	1.50	1.43
2	H	601	NAD	O2B-C2B	2.89	1.50	1.43
2	C	601	NAD	C2N-N1N	2.87	1.38	1.35
2	D	601	NAD	O3D-C3D	-2.82	1.36	1.43
2	A	601	NAD	O3B-C3B	-2.80	1.36	1.43
2	E	601	NAD	O3D-C3D	-2.78	1.36	1.43
2	F	601	NAD	O3D-C3D	-2.77	1.36	1.43
2	G	601	NAD	C8A-N7A	2.75	1.37	1.31
2	F	601	NAD	O2B-C2B	2.75	1.49	1.43
2	F	601	NAD	O3B-C3B	-2.72	1.36	1.43
2	H	601	NAD	C2N-N1N	2.71	1.38	1.35
2	B	601	NAD	O2B-C2B	2.70	1.49	1.43
2	B	601	NAD	C3N-C7N	2.70	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	O3B-C3B	-2.67	1.36	1.43
2	G	601	NAD	O3B-C3B	-2.66	1.36	1.43
2	C	601	NAD	O2B-C2B	2.56	1.49	1.43
2	B	601	NAD	C8A-N7A	2.54	1.36	1.31
2	H	601	NAD	C5A-C4A	-2.52	1.34	1.39
2	D	601	NAD	O2B-C2B	2.51	1.49	1.43
2	F	601	NAD	C5A-C4A	-2.45	1.34	1.39
2	H	601	NAD	O3B-C3B	-2.45	1.36	1.43
2	E	601	NAD	PN-O3	2.44	1.62	1.59
2	A	601	NAD	C8A-N7A	2.42	1.36	1.31
2	B	601	NAD	PN-O3	2.40	1.62	1.59
2	E	601	NAD	C8A-N7A	2.40	1.36	1.31
2	B	601	NAD	C5A-C4A	-2.38	1.34	1.39
2	E	601	NAD	O2B-C2B	2.37	1.48	1.43
2	F	601	NAD	PN-O3	2.37	1.62	1.59
2	B	601	NAD	O2D-C2D	2.33	1.48	1.43
2	F	601	NAD	O2D-C2D	2.33	1.48	1.43
2	D	601	NAD	C5A-C4A	-2.33	1.34	1.39
2	E	601	NAD	O2D-C2D	2.31	1.48	1.43
2	C	601	NAD	C8A-N7A	2.30	1.36	1.31
2	E	601	NAD	C5A-C4A	-2.29	1.35	1.39
2	A	601	NAD	PN-O3	2.28	1.62	1.59
2	G	601	NAD	O2D-C2D	2.27	1.48	1.43
2	C	601	NAD	O3B-C3B	-2.26	1.37	1.43
2	A	601	NAD	O2B-C2B	2.26	1.48	1.43
2	E	601	NAD	O3B-C3B	-2.23	1.37	1.43
2	F	601	NAD	C8A-N7A	2.20	1.35	1.31
2	D	601	NAD	O3B-C3B	-2.19	1.37	1.43
2	C	601	NAD	PA-O3	2.12	1.61	1.59
2	C	601	NAD	O2D-C2D	2.12	1.48	1.43
2	D	601	NAD	O2D-C2D	2.07	1.48	1.43
2	F	601	NAD	C5A-N7A	-2.05	1.35	1.39
2	A	601	NAD	O2D-C2D	2.05	1.48	1.43
2	A	601	NAD	C5A-C4A	-2.04	1.35	1.39
2	D	601	NAD	C5A-N7A	-2.04	1.35	1.39
2	E	601	NAD	PA-O3	2.03	1.61	1.59
2	D	601	NAD	C8A-N7A	2.02	1.35	1.31

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	601	NAD	N3A-C2A-N1A	-5.93	119.60	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	NAD	N3A-C2A-N1A	-5.66	120.01	128.58
2	A	601	NAD	N3A-C2A-N1A	-5.64	120.05	128.58
2	C	601	NAD	C5A-C4A-N3A	-5.55	119.08	126.72
2	B	601	NAD	N3A-C2A-N1A	-5.49	120.27	128.58
2	D	601	NAD	C5A-C4A-N3A	-5.47	119.18	126.72
2	D	601	NAD	N3A-C2A-N1A	-5.42	120.38	128.58
2	H	601	NAD	N3A-C2A-N1A	-5.40	120.40	128.58
2	C	601	NAD	N3A-C2A-N1A	-5.37	120.46	128.58
2	E	601	NAD	N3A-C2A-N1A	-5.36	120.46	128.58
2	B	601	NAD	C5A-C4A-N3A	-5.32	119.40	126.72
2	A	601	NAD	C5A-C4A-N3A	-4.86	120.03	126.72
2	H	601	NAD	C5A-C4A-N3A	-4.77	120.15	126.72
2	E	601	NAD	C5A-C4A-N3A	-4.68	120.27	126.72
2	A	601	NAD	N9A-C8A-N7A	-4.65	107.33	113.94
2	F	601	NAD	C5A-C4A-N3A	-4.64	120.33	126.72
2	H	601	NAD	N9A-C8A-N7A	-4.60	107.41	113.94
2	G	601	NAD	C5A-C4A-N3A	-4.56	120.44	126.72
2	C	601	NAD	N9A-C8A-N7A	-4.46	107.61	113.94
2	F	601	NAD	N9A-C8A-N7A	-4.42	107.66	113.94
2	B	601	NAD	N9A-C8A-N7A	-4.30	107.84	113.94
2	H	601	NAD	C4D-O4D-C1D	-4.24	106.04	109.92
2	G	601	NAD	N9A-C8A-N7A	-4.19	108.00	113.94
2	D	601	NAD	N9A-C8A-N7A	-4.16	108.03	113.94
2	E	601	NAD	N9A-C8A-N7A	-4.14	108.06	113.94
2	F	601	NAD	C4D-O4D-C1D	-3.67	106.56	109.92
2	B	601	NAD	C2A-N3A-C4A	3.63	120.71	111.83
2	F	601	NAD	C3N-C7N-N7N	3.63	122.21	117.74
2	C	601	NAD	C2A-N3A-C4A	3.63	120.69	111.83
2	E	601	NAD	C4D-O4D-C1D	-3.43	106.79	109.92
2	D	601	NAD	C2A-N3A-C4A	3.42	120.18	111.83
2	G	601	NAD	C2A-N3A-C4A	3.39	120.11	111.83
2	D	601	NAD	N3A-C4A-N9A	3.38	132.92	127.17
2	A	601	NAD	C2A-N3A-C4A	3.36	120.03	111.83
2	E	601	NAD	C3N-C7N-N7N	3.31	121.81	117.74
2	H	601	NAD	C2A-N3A-C4A	3.24	119.74	111.83
2	C	601	NAD	C5A-N7A-C8A	3.24	108.54	103.45
2	G	601	NAD	C3N-C7N-N7N	3.24	121.73	117.74
2	C	601	NAD	N3A-C4A-N9A	3.22	132.65	127.17
2	F	601	NAD	C2A-N3A-C4A	3.21	119.67	111.83
2	A	601	NAD	C5A-N7A-C8A	3.13	108.37	103.45
2	H	601	NAD	N3A-C4A-N9A	3.13	132.50	127.17
2	D	601	NAD	C5A-N7A-C8A	3.10	108.33	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	NAD	C2A-N3A-C4A	3.09	119.39	111.83
2	B	601	NAD	C5A-N7A-C8A	3.09	108.30	103.45
2	H	601	NAD	C5A-N7A-C8A	3.02	108.20	103.45
2	B	601	NAD	C4D-O4D-C1D	-3.01	107.17	109.92
2	H	601	NAD	C4A-N9A-C8A	2.93	108.81	105.74
2	A	601	NAD	N3A-C4A-N9A	2.88	132.07	127.17
2	F	601	NAD	C5A-N7A-C8A	2.87	107.96	103.45
2	B	601	NAD	C2N-C3N-C4N	2.86	121.59	118.26
2	C	601	NAD	C4A-C5A-N7A	-2.83	107.34	110.58
2	E	601	NAD	O2N-PN-O3	2.80	114.83	107.27
2	B	601	NAD	C5A-C4A-N9A	2.79	108.85	105.81
2	D	601	NAD	C6A-C5A-C4A	2.78	120.97	117.18
2	F	601	NAD	N3A-C4A-N9A	2.76	131.87	127.17
2	C	601	NAD	C4D-O4D-C1D	-2.76	107.40	109.92
2	E	601	NAD	C5A-N7A-C8A	2.74	107.76	103.45
2	A	601	NAD	C4A-N9A-C8A	2.70	108.57	105.74
2	B	601	NAD	N3A-C4A-N9A	2.69	131.75	127.17
2	B	601	NAD	C4A-C5A-N7A	-2.65	107.55	110.58
2	G	601	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
2	A	601	NAD	C3N-C7N-N7N	2.60	120.94	117.74
2	G	601	NAD	N3A-C4A-N9A	2.58	131.56	127.17
2	G	601	NAD	C4A-N9A-C8A	2.56	108.43	105.74
2	E	601	NAD	N3A-C4A-N9A	2.48	131.39	127.17
2	G	601	NAD	C5A-N7A-C8A	2.47	107.33	103.45
2	A	601	NAD	C6N-N1N-C2N	-2.43	119.81	121.88
2	A	601	NAD	C4A-C5A-N7A	-2.42	107.82	110.58
2	D	601	NAD	C3N-C7N-N7N	2.41	120.71	117.74
2	C	601	NAD	C4A-N9A-C8A	2.37	108.23	105.74
2	D	601	NAD	C4D-O4D-C1D	-2.34	107.78	109.92
2	F	601	NAD	C4A-N9A-C8A	2.34	108.19	105.74
2	E	601	NAD	C5A-C4A-N9A	2.32	108.34	105.81
2	D	601	NAD	C6N-N1N-C2N	-2.32	119.91	121.88
2	E	601	NAD	C4A-C5A-N7A	-2.29	107.96	110.58
2	D	601	NAD	C4A-C5A-N7A	-2.29	107.96	110.58
2	C	601	NAD	C5A-C4A-N9A	2.26	108.27	105.81
2	F	601	NAD	O7N-C7N-C3N	-2.25	116.85	119.60
2	H	601	NAD	C2N-C3N-C4N	2.21	120.82	118.26
2	C	601	NAD	C2N-C3N-C4N	2.20	120.81	118.26
2	A	601	NAD	C4D-O4D-C1D	-2.11	107.99	109.92
2	A	601	NAD	O2N-PN-O3	2.11	112.97	107.27
2	F	601	NAD	C6A-C5A-C4A	2.11	120.05	117.18
2	C	601	NAD	C6A-C5A-C4A	2.10	120.05	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	NAD	C6A-C5A-C4A	2.08	120.02	117.18
2	H	601	NAD	C4A-C5A-N7A	-2.06	108.23	110.58
2	E	601	NAD	C6A-C5A-C4A	2.06	119.99	117.18
2	G	601	NAD	C4A-C5A-N7A	-2.04	108.25	110.58
2	E	601	NAD	C4A-N9A-C8A	2.04	107.88	105.74
2	C	601	NAD	N6A-C6A-N1A	-2.04	113.84	118.38
2	C	601	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
2	E	601	NAD	C2N-C3N-C4N	2.02	120.61	118.26
2	B	601	NAD	C6A-C5A-C4A	2.02	119.93	117.18
2	G	601	NAD	C5A-C4A-N9A	2.01	108.00	105.81
2	A	601	NAD	C6A-C5A-C4A	2.01	119.92	117.18

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	603	PGE	C3-C4-O3-C5
5	D	604	PGE	C4-C3-O2-C2
4	A	604	PG4	C3-C4-O3-C5
4	H	602	PG4	C6-C5-O3-C4
4	A	604	PG4	O2-C3-C4-O3
5	F	603	PGE	O3-C5-C6-O4
5	A	606	PGE	O2-C3-C4-O3
4	A	604	PG4	C1-C2-O2-C3
4	A	604	PG4	O4-C7-C8-O5
4	E	604	PG4	O1-C1-C2-O2
4	F	602	PG4	O4-C7-C8-O5
5	A	606	PGE	O3-C5-C6-O4
5	H	603	PGE	O1-C1-C2-O2
5	F	603	PGE	O2-C3-C4-O3
7	C	605	1PE	OH5-C14-C24-OH4
5	A	606	PGE	O1-C1-C2-O2
5	B	603	PGE	O1-C1-C2-O2
5	F	603	PGE	O1-C1-C2-O2
5	F	604	PGE	O3-C5-C6-O4
5	F	604	PGE	O2-C3-C4-O3
5	E	606	PGE	O2-C3-C4-O3
5	E	605	PGE	O2-C3-C4-O3
4	D	603	PG4	O4-C7-C8-O5
4	H	602	PG4	O1-C1-C2-O2
5	E	606	PGE	O1-C1-C2-O2
4	H	602	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	H	602	PG4	C8-C7-O4-C6
4	E	604	PG4	O4-C7-C8-O5
5	E	605	PGE	O1-C1-C2-O2
6	E	607	EDO	O1-C1-C2-O2
5	H	603	PGE	O2-C3-C4-O3
4	D	603	PG4	O1-C1-C2-O2
4	H	602	PG4	O4-C7-C8-O5
5	C	603	PGE	O3-C5-C6-O4
5	G	606	PGE	O1-C1-C2-O2
5	D	604	PGE	O2-C3-C4-O3
5	B	603	PGE	O3-C5-C6-O4
5	D	604	PGE	O1-C1-C2-O2
5	G	604	PGE	O3-C5-C6-O4
4	D	603	PG4	C6-C5-O3-C4
4	E	604	PG4	O3-C5-C6-O4
4	A	604	PG4	O1-C1-C2-O2
2	B	601	NAD	C2B-C1B-N9A-C8A
2	D	601	NAD	C2B-C1B-N9A-C8A
2	E	601	NAD	C2B-C1B-N9A-C8A
2	F	601	NAD	C2B-C1B-N9A-C8A
5	B	603	PGE	O2-C3-C4-O3
2	B	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C4D-C5D-O5D-PN
2	G	601	NAD	C4D-C5D-O5D-PN
5	G	604	PGE	O2-C3-C4-O3
5	F	604	PGE	C4-C3-O2-C2
2	A	601	NAD	C2B-C1B-N9A-C8A
2	C	601	NAD	C2B-C1B-N9A-C8A
2	G	601	NAD	C2B-C1B-N9A-C8A
2	H	601	NAD	C2B-C1B-N9A-C8A
5	A	605	PGE	C3-C4-O3-C5
5	B	603	PGE	C1-C2-O2-C3
7	C	605	1PE	C12-C22-OH3-C23
2	A	601	NAD	C4D-C5D-O5D-PN
5	E	606	PGE	C3-C4-O3-C5
5	G	604	PGE	C3-C4-O3-C5
5	A	606	PGE	C6-C5-O3-C4
5	C	603	PGE	C3-C4-O3-C5
2	B	601	NAD	C2B-C1B-N9A-C4A
5	D	604	PGE	C1-C2-O2-C3
4	E	604	PG4	C4-C3-O2-C2
5	F	604	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
5	H	603	PGE	C1-C2-O2-C3
2	E	601	NAD	C3D-C4D-C5D-O5D
2	E	601	NAD	C4D-C5D-O5D-PN
4	E	604	PG4	O2-C3-C4-O3
5	A	606	PGE	C1-C2-O2-C3
5	G	605	PGE	O1-C1-C2-O2
5	E	606	PGE	C1-C2-O2-C3
5	E	605	PGE	C6-C5-O3-C4
2	C	601	NAD	C4D-C5D-O5D-PN
2	H	601	NAD	C4D-C5D-O5D-PN
5	F	603	PGE	C4-C3-O2-C2
5	F	604	PGE	C6-C5-O3-C4
2	A	601	NAD	C5B-O5B-PA-O1A
2	G	601	NAD	C5B-O5B-PA-O1A
2	H	601	NAD	C5B-O5B-PA-O1A
2	F	601	NAD	C4D-C5D-O5D-PN
4	A	604	PG4	C5-C6-O4-C7
5	G	606	PGE	O2-C3-C4-O3
4	F	602	PG4	O2-C3-C4-O3
4	E	604	PG4	C8-C7-O4-C6
5	H	603	PGE	O3-C5-C6-O4
7	C	605	1PE	C23-C13-OH4-C24
2	A	601	NAD	C2B-C1B-N9A-C4A
2	C	601	NAD	C2B-C1B-N9A-C4A
2	D	601	NAD	C2B-C1B-N9A-C4A
2	E	601	NAD	C2B-C1B-N9A-C4A
2	F	601	NAD	C2B-C1B-N9A-C4A
2	G	601	NAD	C2B-C1B-N9A-C4A
2	H	601	NAD	C2B-C1B-N9A-C4A
2	F	601	NAD	C3D-C4D-C5D-O5D
6	A	607	EDO	O1-C1-C2-O2
4	D	603	PG4	C4-C3-O2-C2
5	A	606	PGE	C4-C3-O2-C2
5	G	604	PGE	C1-C2-O2-C3
5	E	605	PGE	C4-C3-O2-C2
5	A	606	PGE	C3-C4-O3-C5
4	B	602	PG4	C5-C6-O4-C7
2	A	601	NAD	O4B-C1B-N9A-C8A
5	G	605	PGE	O2-C3-C4-O3
2	E	601	NAD	O4D-C4D-C5D-O5D
5	H	603	PGE	C4-C3-O2-C2
4	D	603	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	C	604	EDO	O1-C1-C2-O2
2	C	601	NAD	O4B-C1B-N9A-C8A
2	D	601	NAD	O4B-C1B-N9A-C8A
2	E	601	NAD	O4B-C1B-N9A-C8A
2	G	601	NAD	O4B-C1B-N9A-C8A
2	H	601	NAD	O4B-C1B-N9A-C8A
7	C	605	1PE	C13-C23-OH3-C22
2	B	601	NAD	O4B-C1B-N9A-C8A
2	F	601	NAD	O4B-C1B-N9A-C8A
5	E	605	PGE	O3-C5-C6-O4

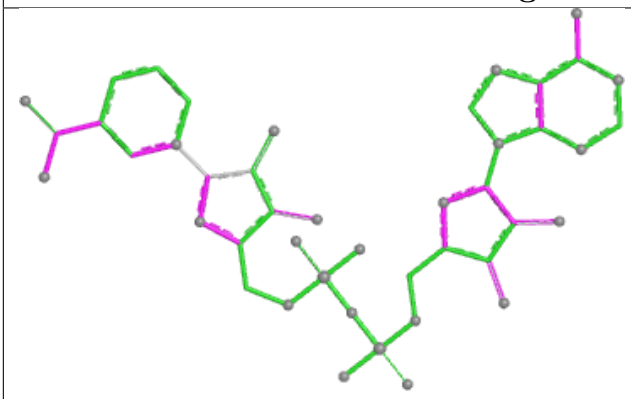
There are no ring outliers.

14 monomers are involved in 18 short contacts:

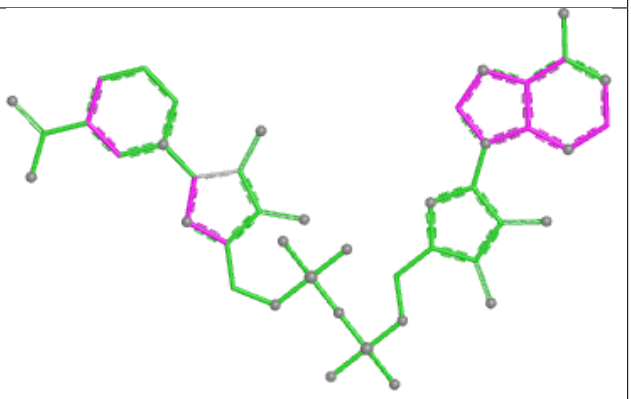
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	601	NAD	1	0
2	A	601	NAD	1	0
5	H	603	PGE	1	0
5	F	603	PGE	1	0
2	G	601	NAD	1	0
2	B	601	NAD	1	0
4	E	604	PG4	3	0
5	G	605	PGE	1	0
4	A	604	PG4	1	0
5	E	606	PGE	1	0
5	F	604	PGE	1	0
4	H	602	PG4	1	0
5	G	606	PGE	2	0
5	A	606	PGE	2	0

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 then 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.

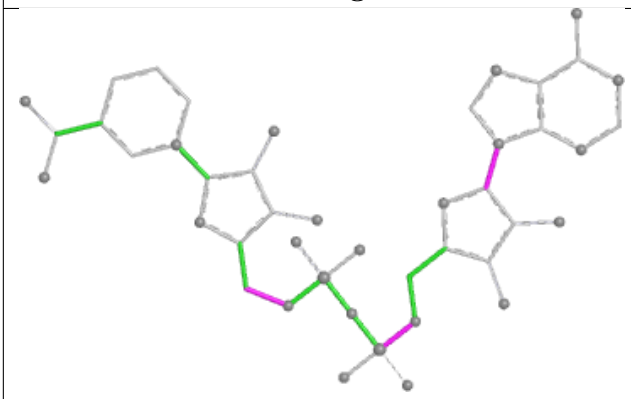
Ligand NAD H 601



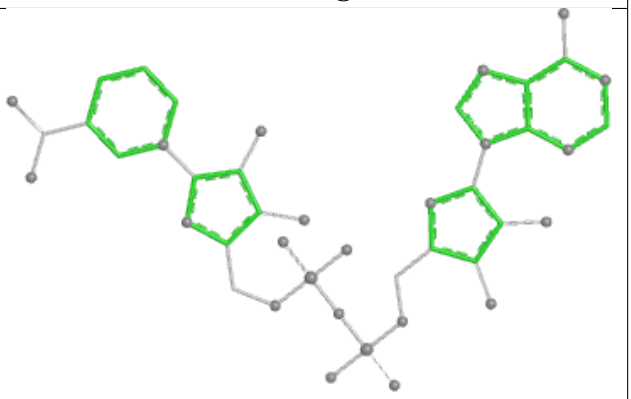
Bond lengths



Bond angles

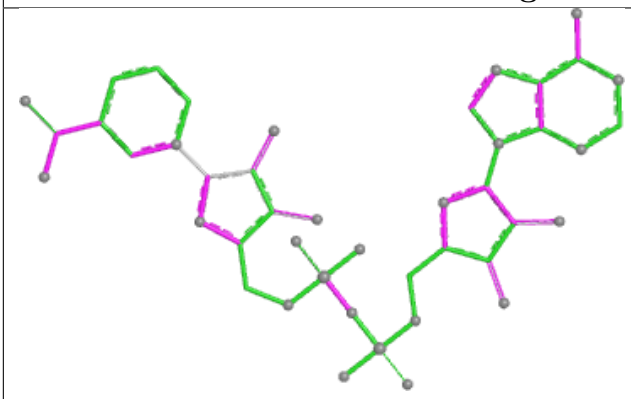


Torsions



Rings

Ligand NAD A 601



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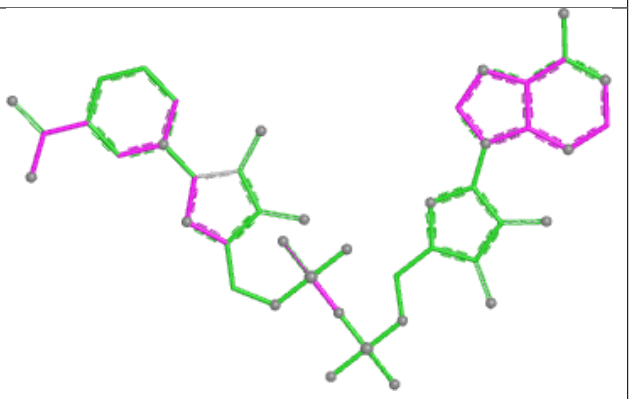

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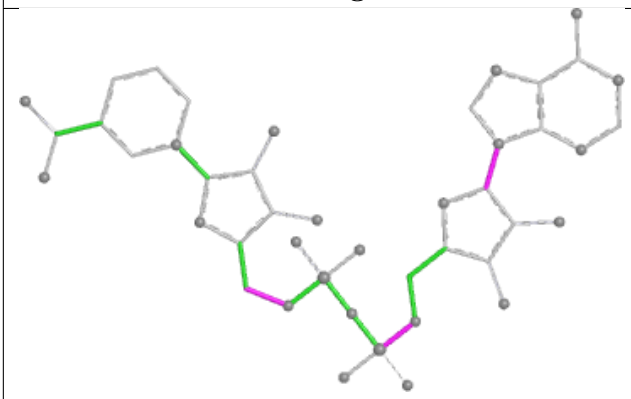

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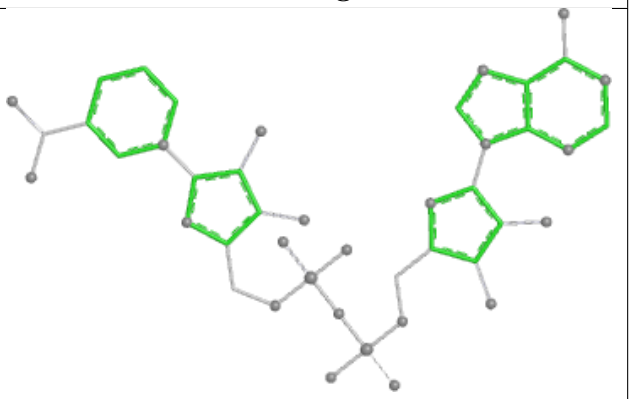
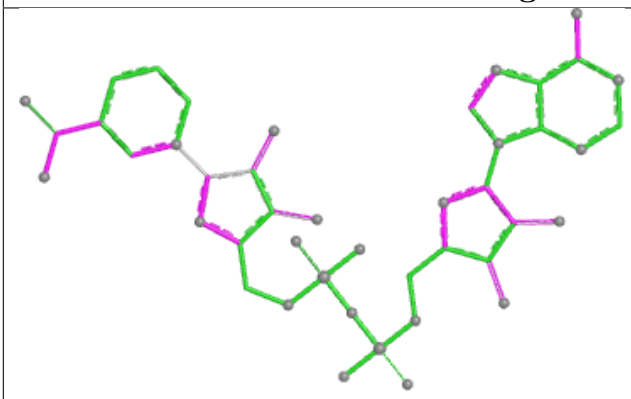
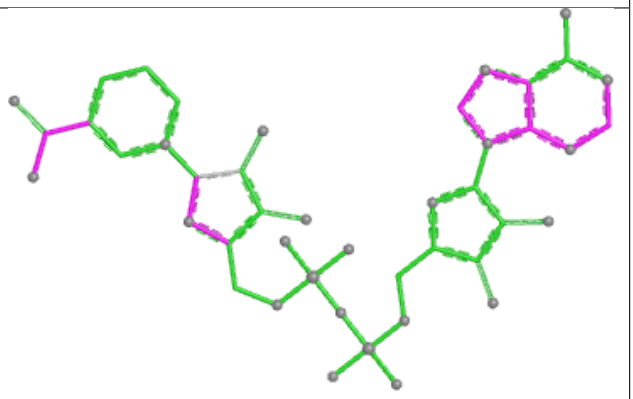


Rings

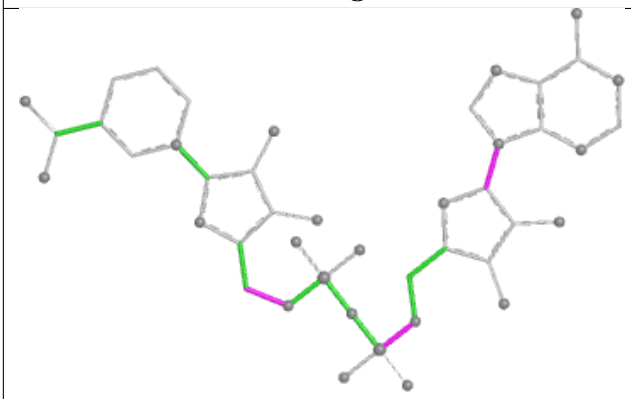
Ligand NAD G 601



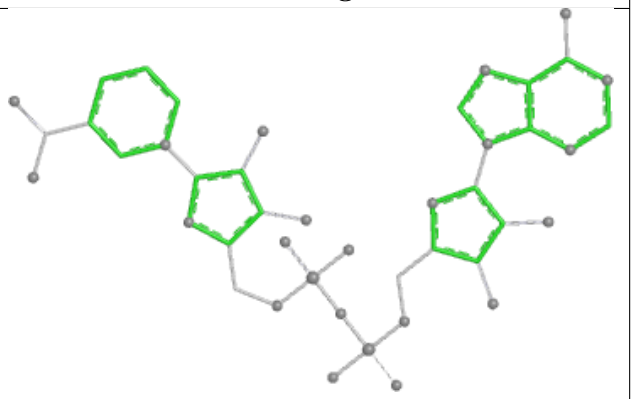
Bond lengths



Bond angles

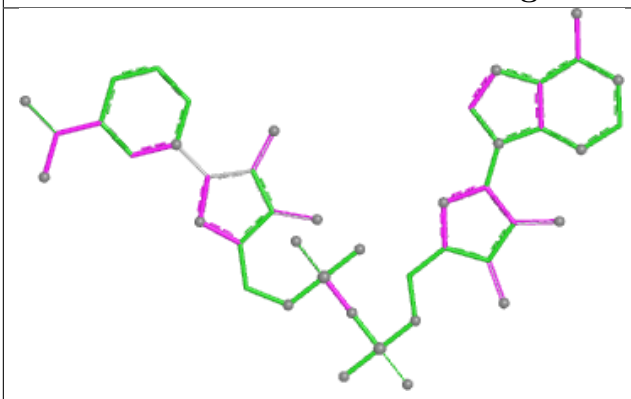


Torsions



Rings

Ligand NAD B 601



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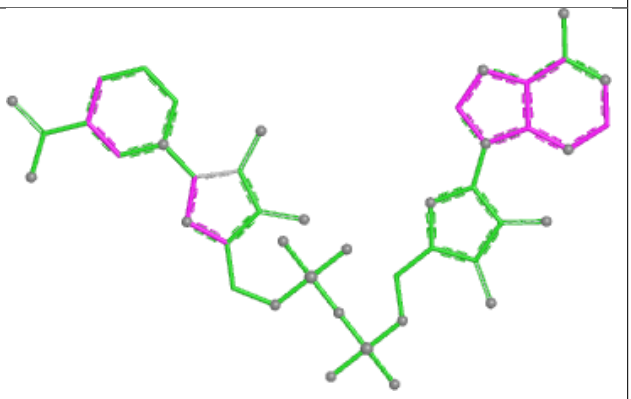

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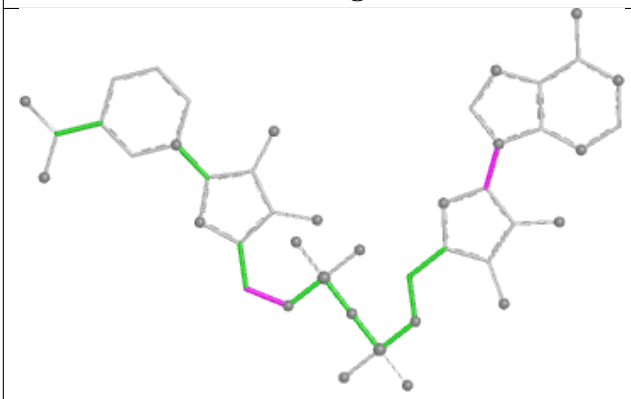

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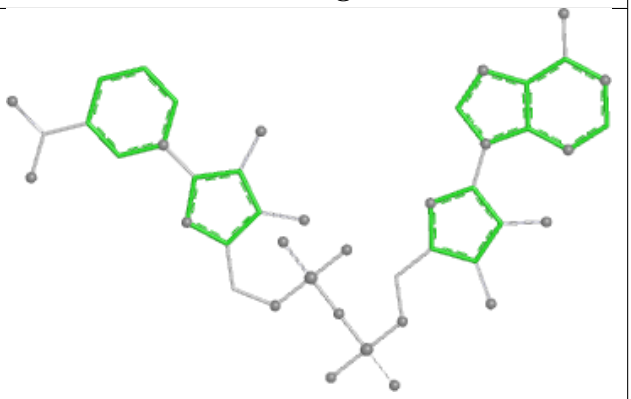
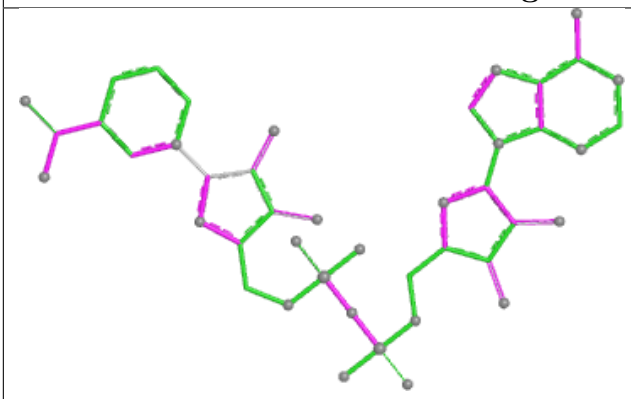


Rings

Ligand NAD E 601



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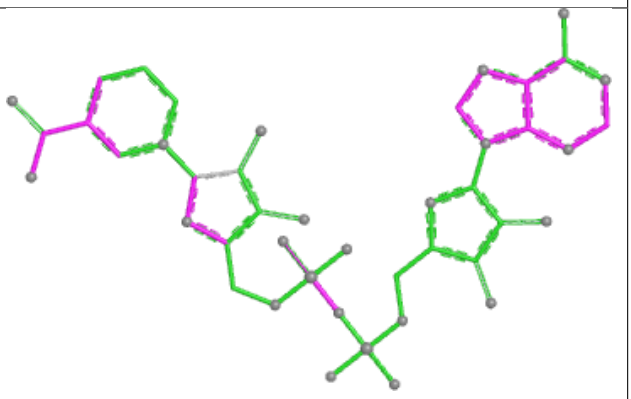

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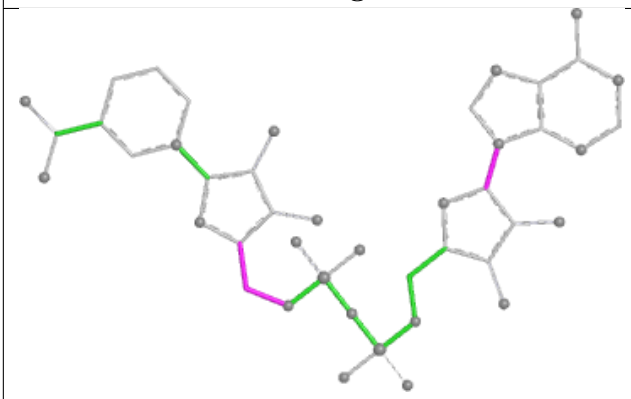

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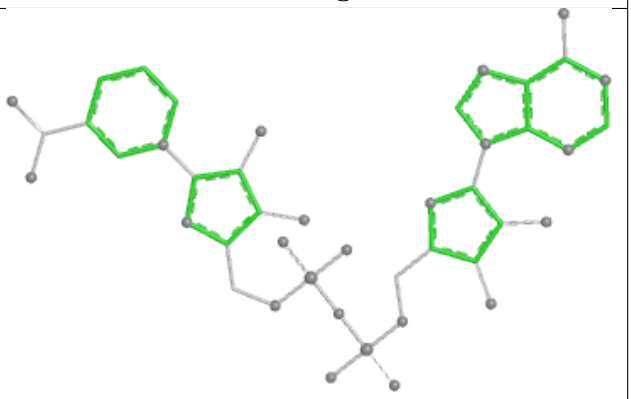
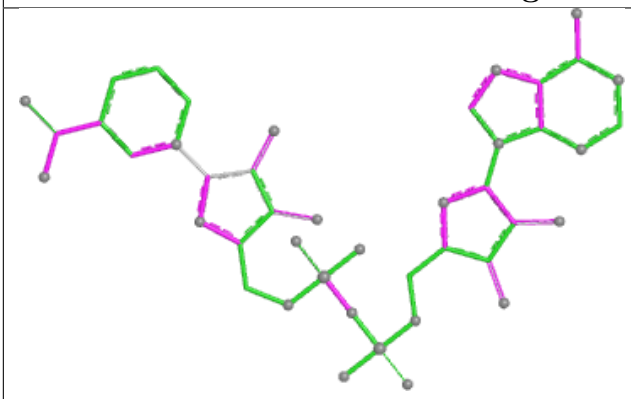


Rings

Ligand NAD F 601



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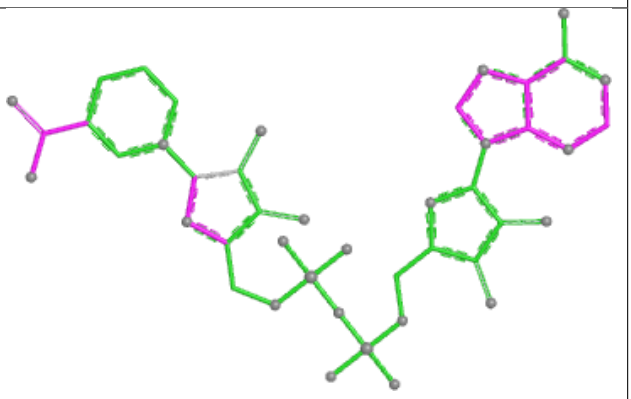
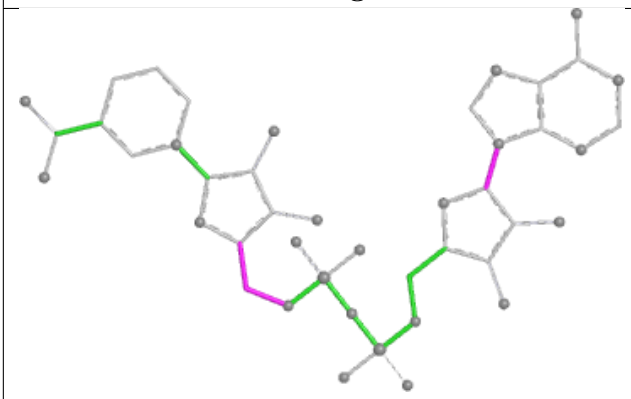
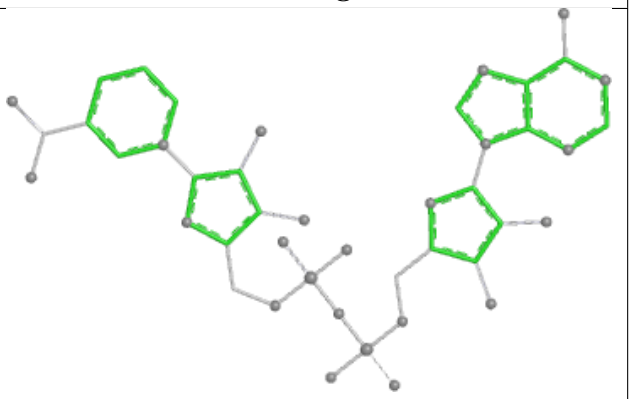


Bond angles

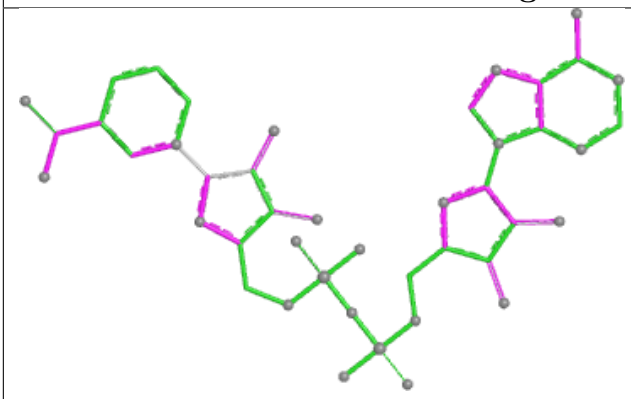


Torsions

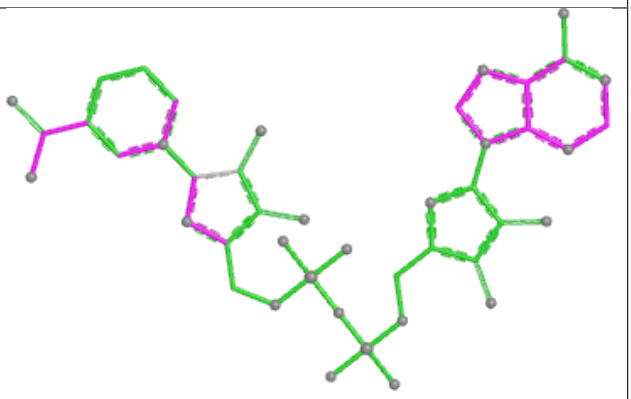


Rings

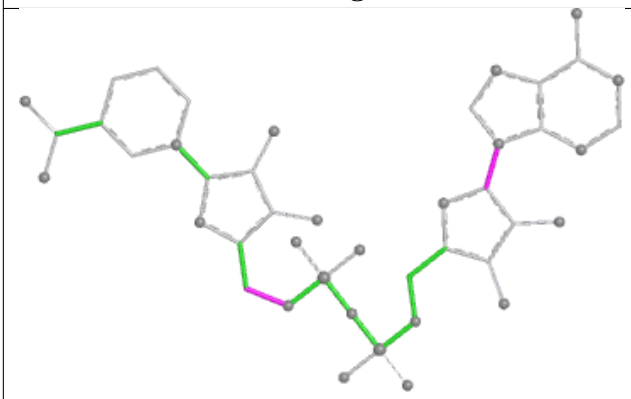
Ligand NAD D 601



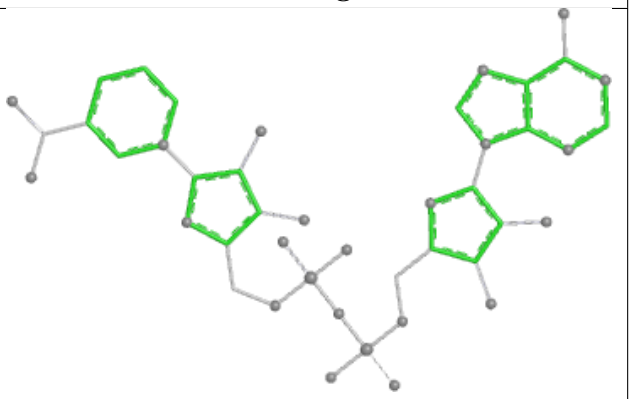
Bond lengths



Bond angles

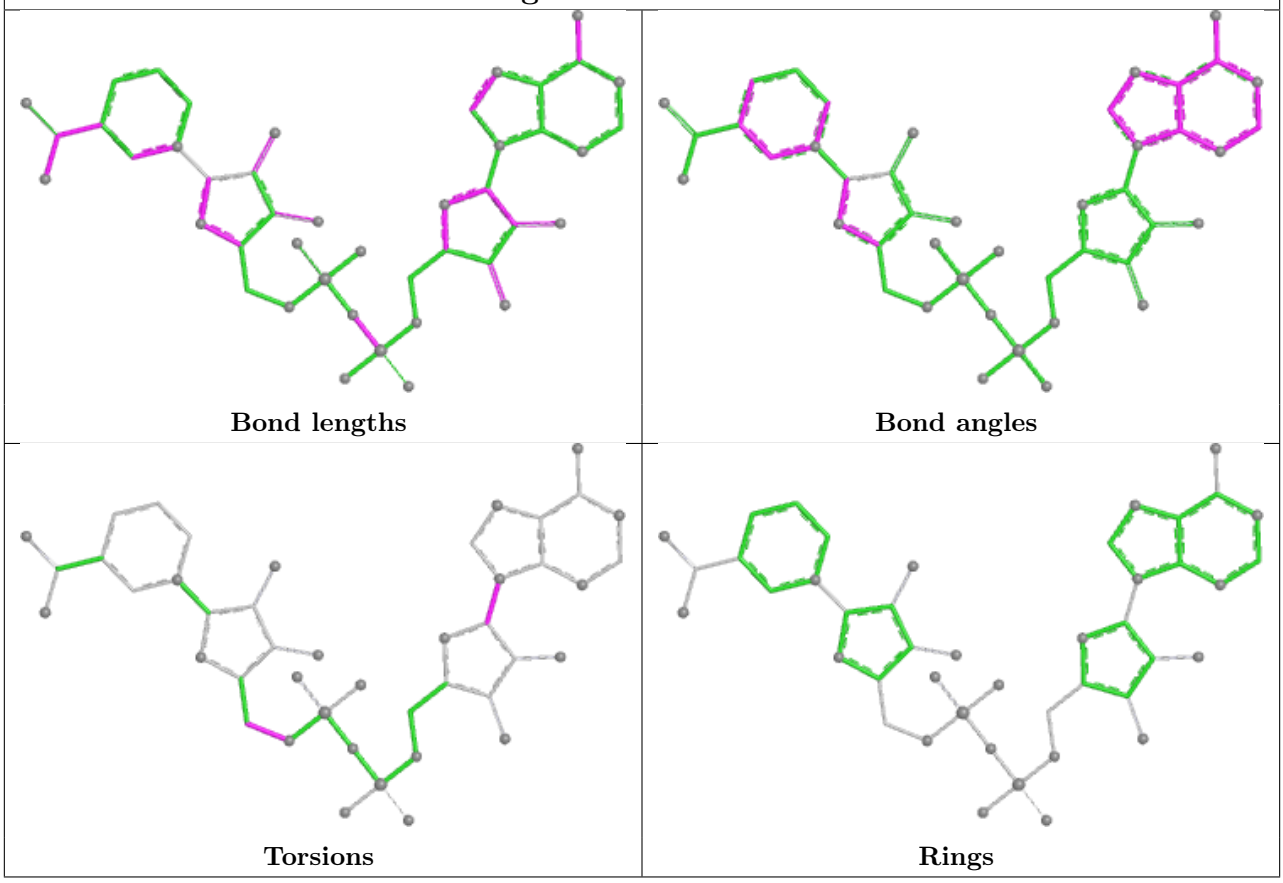


Torsions



Rings

Ligand NAD C 601



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	509/513 (99%)	-0.44	1 (0%)	91	93	9, 23, 38, 60	2 (0%)
1	B	509/513 (99%)	-0.35	3 (0%)	85	88	11, 24, 42, 55	2 (0%)
1	C	509/513 (99%)	-0.35	3 (0%)	85	88	10, 24, 45, 67	1 (0%)
1	D	509/513 (99%)	-0.33	2 (0%)	88	91	10, 26, 44, 55	3 (0%)
1	E	509/513 (99%)	-0.43	1 (0%)	91	93	13, 24, 39, 49	3 (0%)
1	F	509/513 (99%)	-0.36	4 (0%)	82	86	13, 23, 41, 63	1 (0%)
1	G	509/513 (99%)	-0.33	8 (1%)	70	74	12, 25, 41, 79	3 (0%)
1	H	509/513 (99%)	-0.40	2 (0%)	88	91	11, 25, 40, 57	1 (0%)
All	All	4072/4104 (99%)	-0.37	24 (0%)	85	88	9, 24, 42, 79	16 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	510	PHE	3.6
1	F	335	TRP	3.4
1	G	505	ALA	3.4
1	E	292[A]	PHE	3.1
1	G	502	LEU	2.8
1	D	337	PRO	2.7
1	G	504	LEU	2.6
1	B	335	TRP	2.6
1	G	503	PRO	2.6
1	F	504	LEU	2.5
1	F	3	THR	2.5
1	F	331	VAL	2.5
1	B	505	ALA	2.4
1	G	508	ILE	2.4
1	D	338	ASN	2.3
1	H	462	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	335	TRP	2.3
1	G	507	GLY	2.2
1	C	394	SER	2.1
1	B	3	THR	2.1
1	G	509	LYS	2.1
1	H	337	PRO	2.1
1	C	504	LEU	2.1
1	A	3	THR	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
6	EDO	C	604	4/4	0.78	0.14	52,53,56,61	0
5	PGE	E	605	10/10	0.81	0.14	44,48,49,51	0
6	EDO	E	607	4/4	0.81	0.14	34,35,39,50	0
5	PGE	E	606	10/10	0.82	0.16	49,55,57,59	0
4	PG4	E	604	13/13	0.84	0.14	38,43,47,47	0
5	PGE	C	603	10/10	0.85	0.15	40,49,56,57	0
5	PGE	D	604	10/10	0.85	0.14	45,52,55,56	0
5	PGE	A	605	10/10	0.87	0.13	42,50,54,55	0
6	EDO	D	605	4/4	0.87	0.11	38,39,44,44	0
6	EDO	D	606	4/4	0.87	0.14	41,42,42,42	0
5	PGE	G	605	7/10	0.87	0.13	32,37,42,52	0
5	PGE	F	603	10/10	0.88	0.13	45,49,56,56	0
5	PGE	G	604	10/10	0.88	0.13	36,48,51,54	0
5	PGE	B	603	10/10	0.88	0.13	40,45,53,53	0
5	PGE	G	606	10/10	0.88	0.13	42,48,50,53	0

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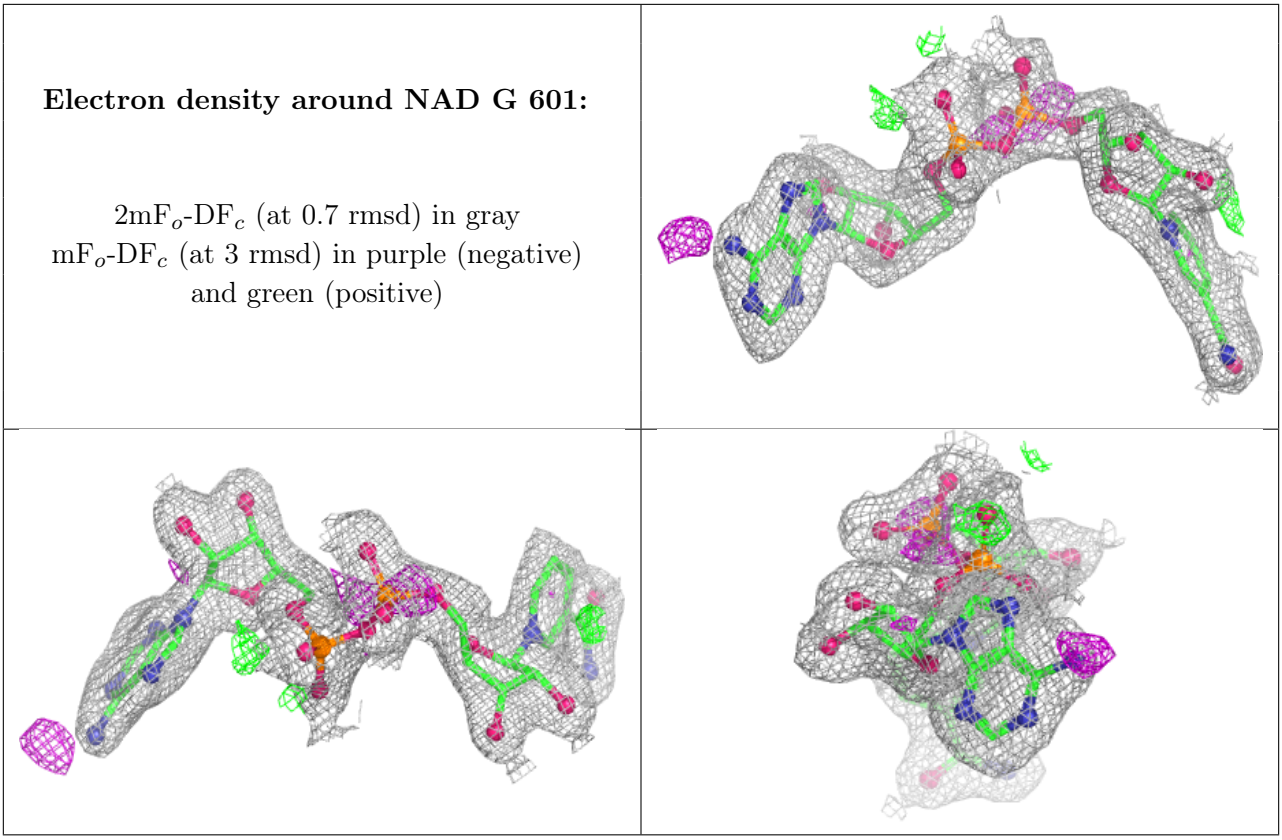
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	A	606	10/10	0.89	0.11	42,48,55,58	0
5	PGE	H	603	10/10	0.89	0.12	43,48,49,52	0
6	EDO	A	607	4/4	0.90	0.12	38,42,46,46	0
4	PG4	D	603	13/13	0.91	0.10	25,34,42,44	0
4	PG4	A	604	13/13	0.92	0.10	27,38,41,45	0
4	PG4	H	602	13/13	0.92	0.10	29,37,40,41	0
5	PGE	F	604	10/10	0.92	0.09	38,43,47,49	0
3	CL	D	602	1/1	0.93	0.09	46,46,46,46	0
4	PG4	B	602	13/13	0.93	0.10	28,36,44,45	0
5	PGE	H	604	10/10	0.93	0.08	28,32,40,40	0
4	PG4	F	602	13/13	0.93	0.10	30,33,51,56	0
7	1PE	C	605	16/16	0.94	0.08	31,35,46,50	0
3	CL	E	603	1/1	0.95	0.09	44,44,44,44	0
2	NAD	G	601	44/44	0.95	0.07	17,29,34,39	0
2	NAD	A	601	44/44	0.95	0.07	16,25,32,33	0
2	NAD	H	601	44/44	0.96	0.06	17,26,33,36	0
3	CL	A	603	1/1	0.96	0.10	40,40,40,40	0
2	NAD	D	601	44/44	0.96	0.07	21,30,37,39	0
2	NAD	E	601	44/44	0.96	0.06	17,26,33,33	0
2	NAD	F	601	44/44	0.96	0.06	14,28,34,37	0
2	NAD	B	601	44/44	0.96	0.06	17,27,35,39	0
3	CL	G	603	1/1	0.97	0.09	41,41,41,41	0
2	NAD	C	601	44/44	0.97	0.06	17,29,39,41	0
3	CL	G	602	1/1	0.97	0.11	48,48,48,48	0
3	CL	E	602	1/1	0.99	0.05	33,33,33,33	0
3	CL	C	602	1/1	0.99	0.10	41,41,41,41	0
3	CL	A	602	1/1	0.99	0.07	35,35,35,35	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.

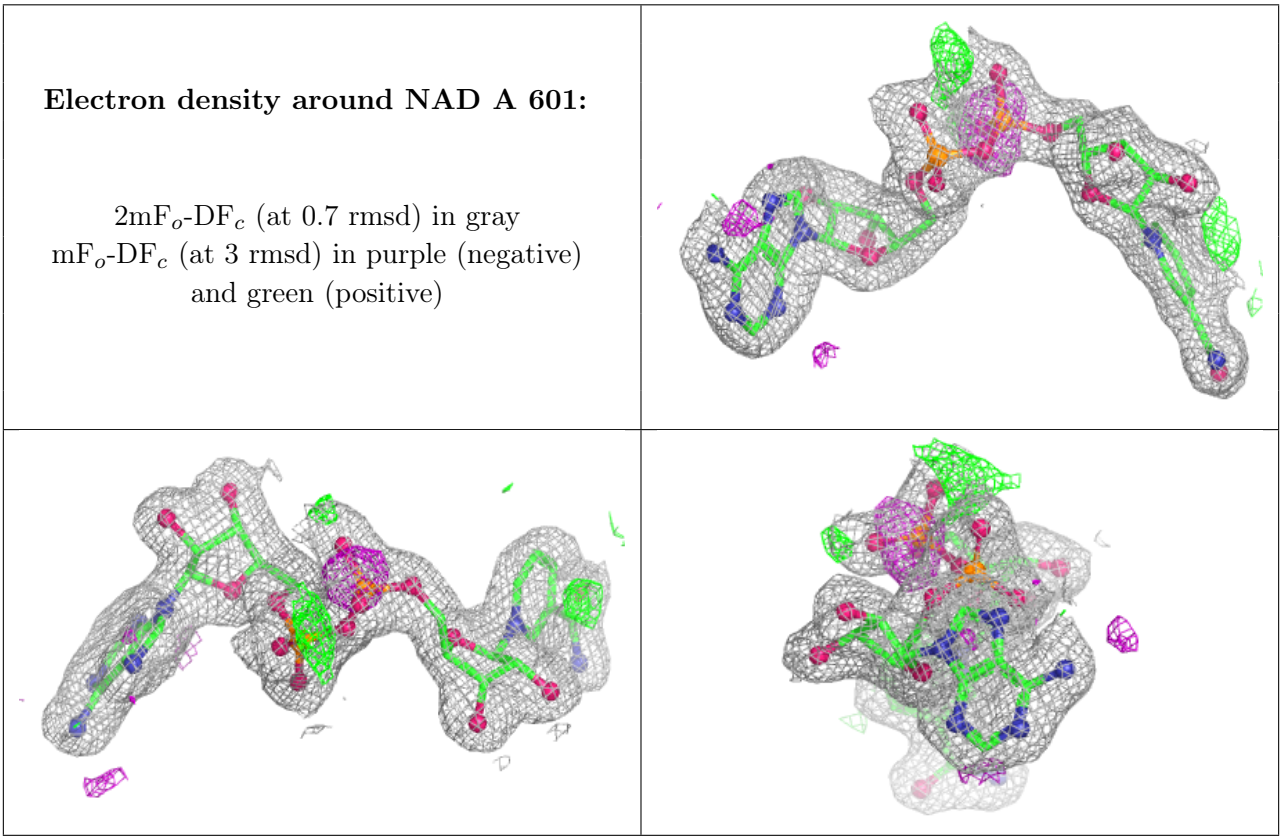
Electron density around NAD G 601:

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



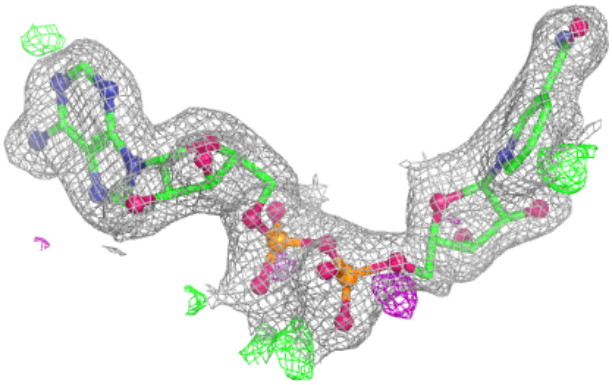
Electron density around NAD A 601:

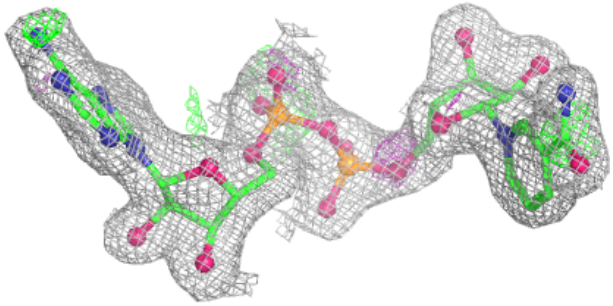
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

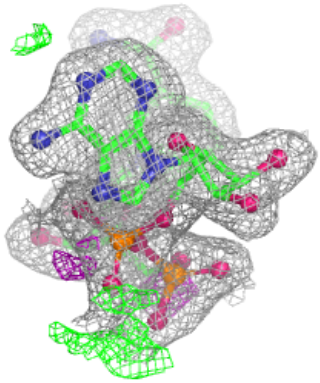


Electron density around NAD H 601:

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

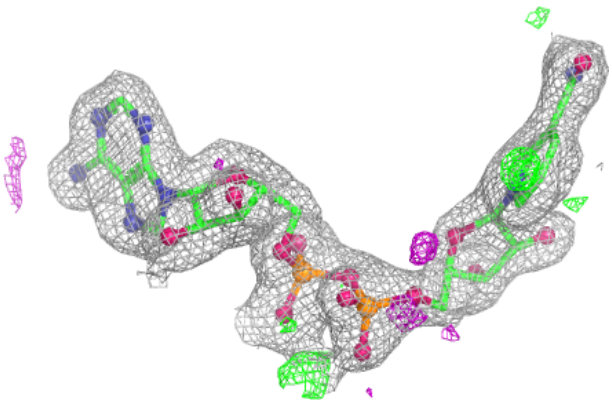


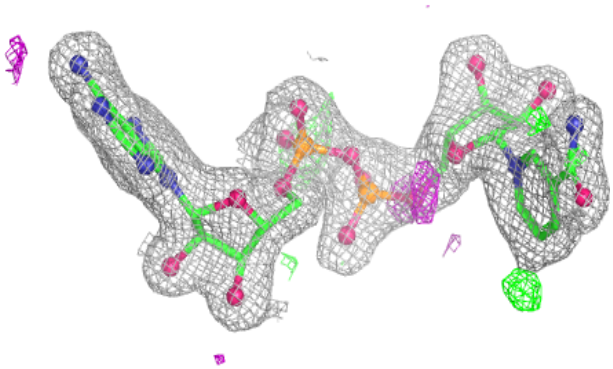


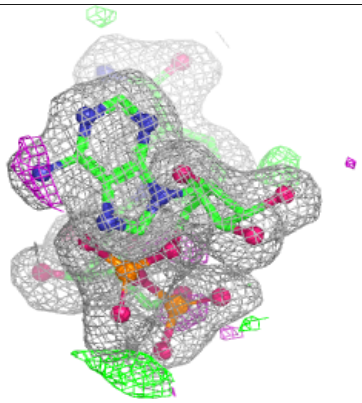


Electron density around NAD D 601:

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

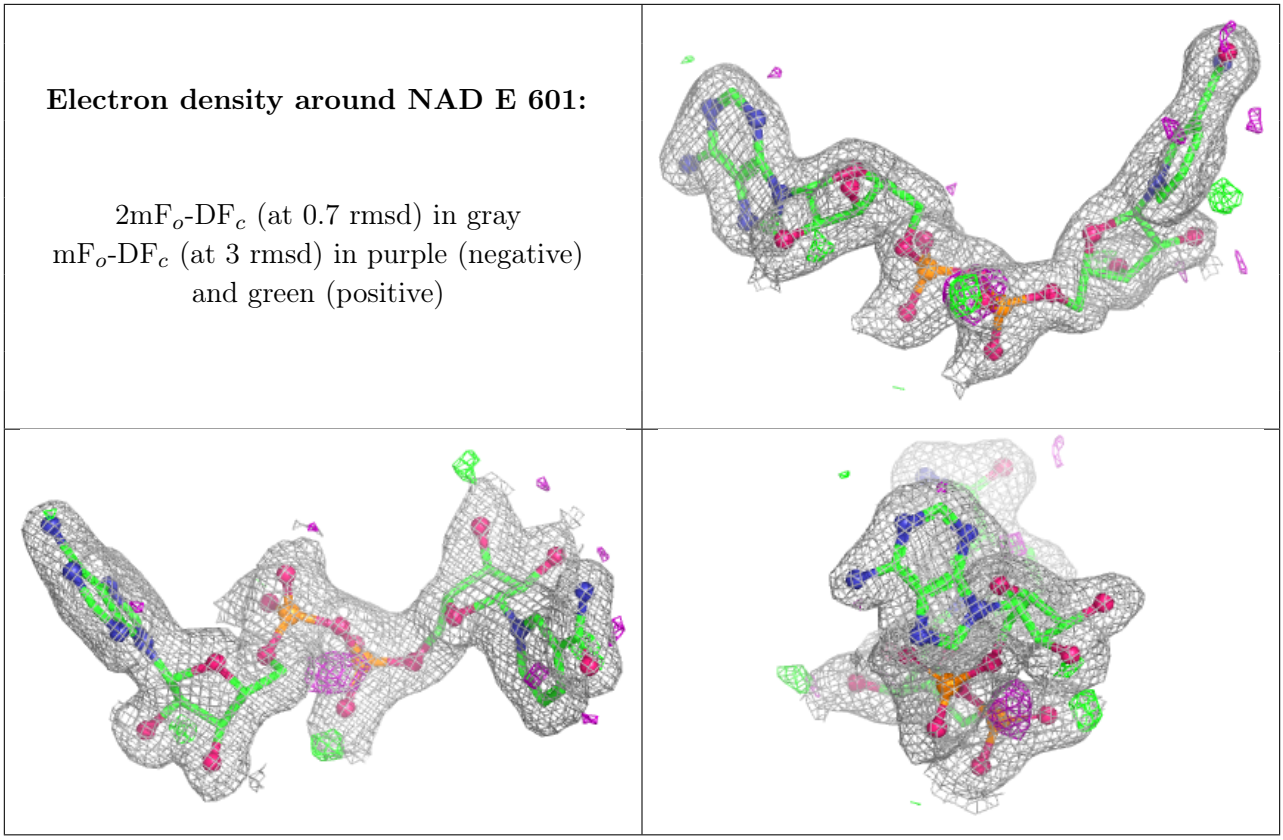






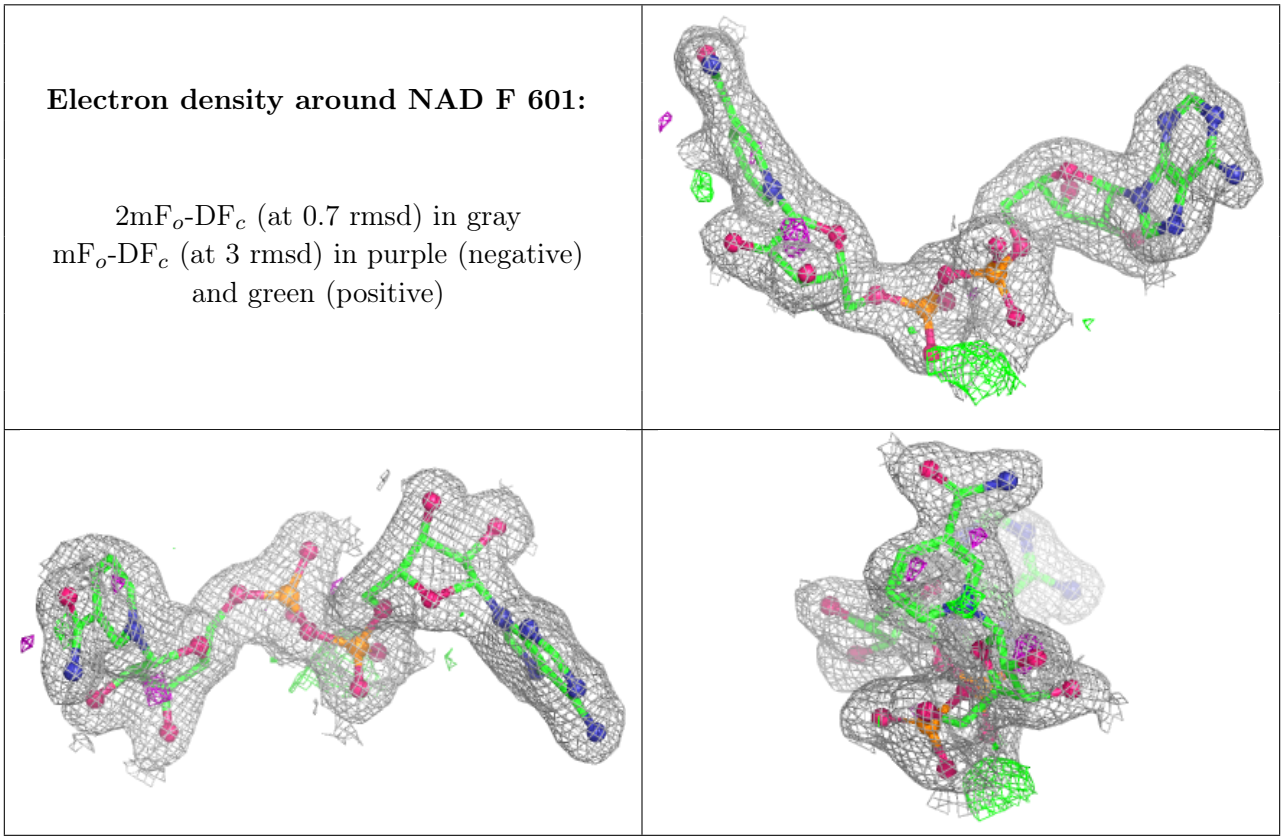
Electron density around NAD E 601:

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



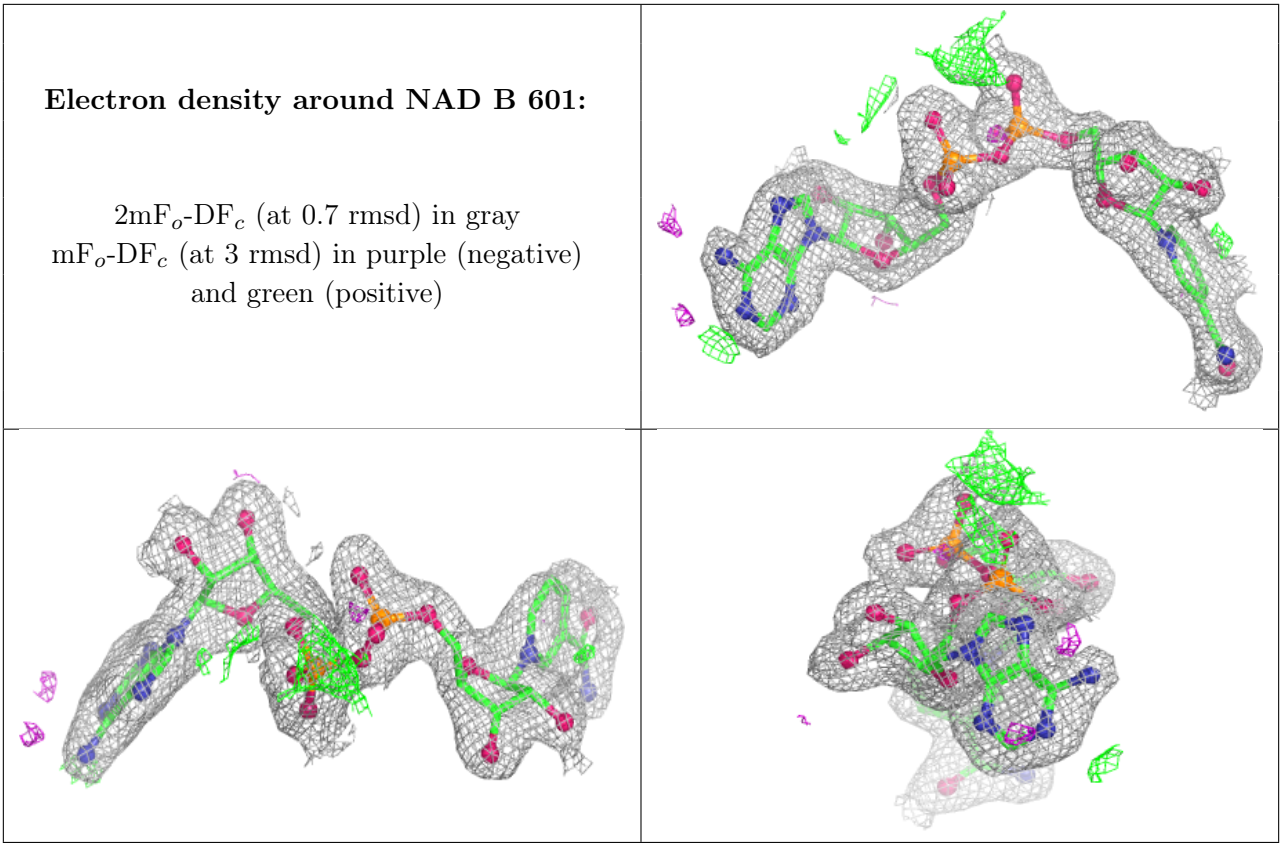
Electron density around NAD F 601:

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



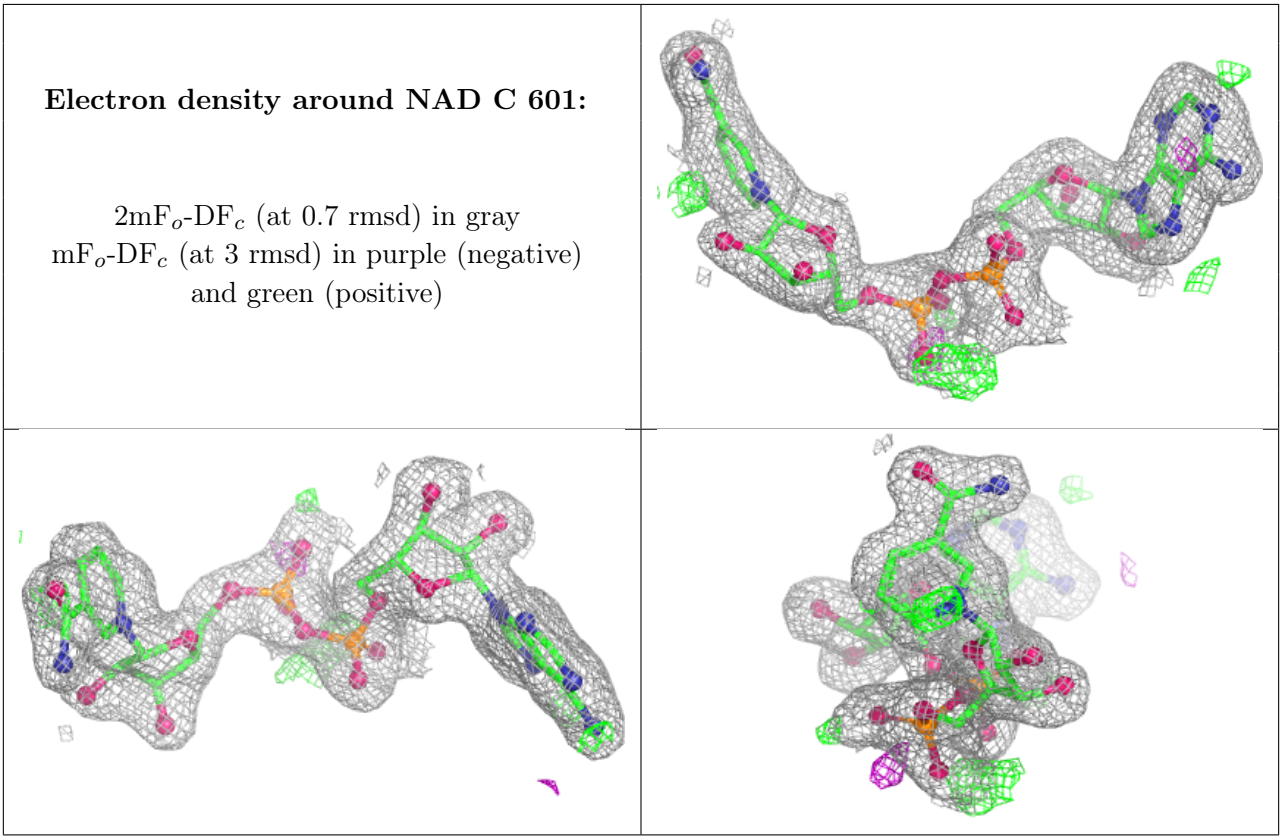
Electron density around NAD B 601:

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



Electron density around NAD C 601:

$2mF_o$-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.