Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 03:11 AM BST

PDB ID	:	6O4K
Title	:	Structure of ALDH7A1 mutant E399Q complexed with NAD
Authors	:	Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on	:	2019-02-28
Resolution	:	2.06 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 following versions of software and data (see references (i)) were used in the production of this report:

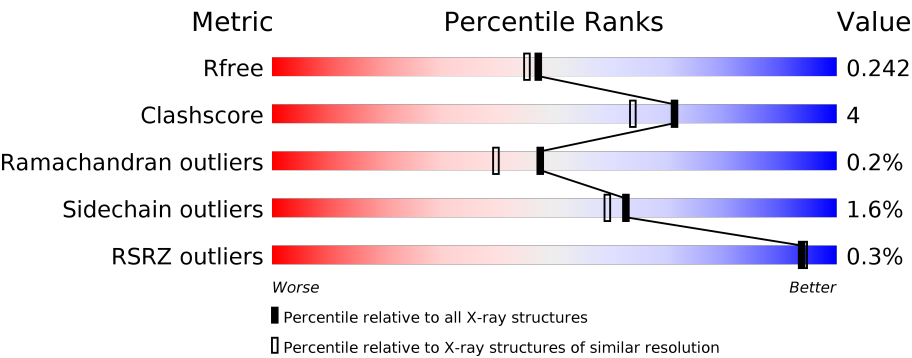|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.06 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		1.6%
RSRZ outliers		0.3%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	91% 9% •
1	B	513	% 90% 9% •
1	C	513	% 87% 12% ••
1	D	513	88% 11% •
1	E	513	91% 8% ••
1	F	513	91% 9% •

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32399 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 3858	C 2450	N 670	O 721	S 17	0	0	0
1	B	509	Total 3867	C 2459	N 673	O 718	S 17	0	1	0
1	C	509	Total 3868	C 2459	N 675	O 717	S 17	0	2	0
1	D	509	Total 3822	C 2430	N 666	O 709	S 17	0	0	0
1	E	509	Total 3864	C 2453	N 670	O 724	S 17	0	1	0
1	F	509	Total 3863	C 2451	N 671	O 724	S 17	0	0	0
1	G	507	Total 3820	C 2426	N 666	O 711	S 17	0	0	0
1	H	509	Total 3839	C 2436	N 670	O 716	S 17	0	0	0

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	399	GLN	GLU	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	399	GLN	GLU	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	399	GLN	GLU	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	399	GLN	GLU	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	399	GLN	GLU	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	399	GLN	GLU	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	399	GLN	GLU	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	399	GLN	GLU	engineered mutation	UNP P49419

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
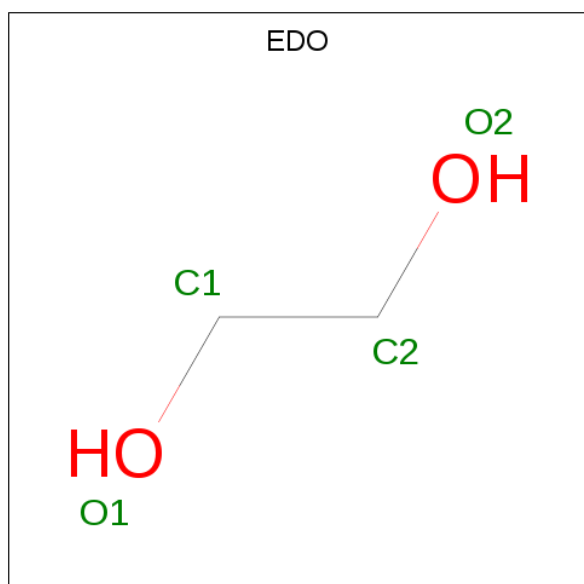
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	C	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	D	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	1
			54	20	10	20	4		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
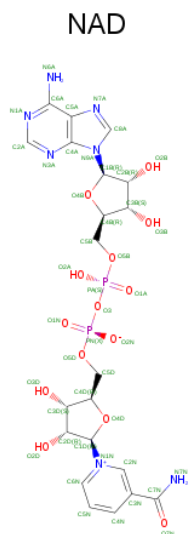
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	2	Total	Cl	0	0
			2	2		
4	H	1	Total	Cl	0	0
			1	1		

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	200	Total 200	O 200	0	0
5	B	136	Total 136	O 136	0	0
5	C	153	Total 153	O 153	0	0
5	D	125	Total 125	O 125	0	0
5	E	173	Total 173	O 173	0	0
5	F	162	Total 162	O 162	0	0
5	G	140	Total 140	O 140	0	0
5	H	161	Total 161	O 161	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

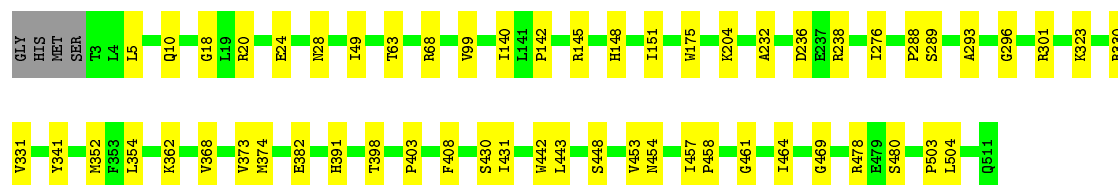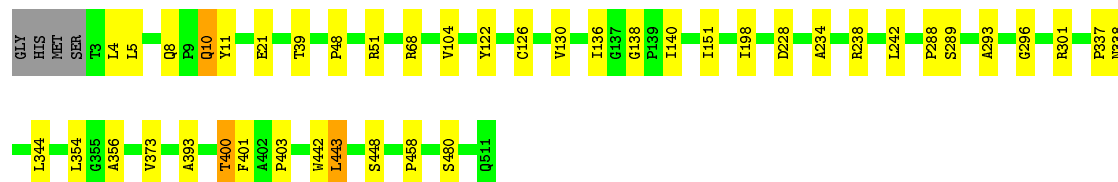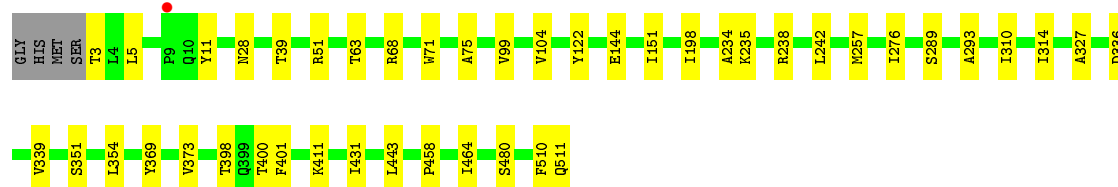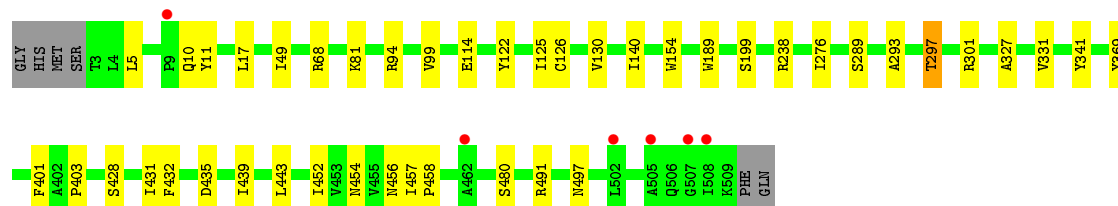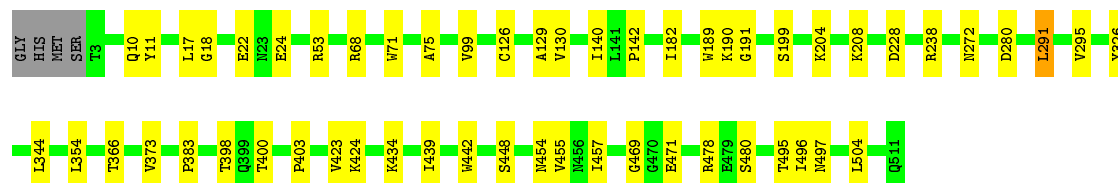Chain A:

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain B:

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain C:

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain D:

GLY HIS MET SER T3 L4 L5 Q10 G18 L19 R20 E24 N28 I49 T63 R68 V99 I140 L141 P142 R145 H148 I151 W175 K204 A232 D236 E237 R238 I276 P288 S289 A293 G296 R301 K323 R330

V331 Y341 M352 F353 L354 K362 V368 V373 M374 E382 H391 T398 P403 F408 S430 I431 W442 L443 S448 V453 N454 I457 P458 G461 I464 G469 I464 R478 E479 S480 P503 L504 Q511

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain E: 91% 8%

GLY HIS MET SER T3 L4 L5 Q8 P9 Q10 Y11 E21 T39 P48 R51 T39 R68 V104 Y122 C126 V130 I136 G137 G138 P139 I140 I151 I198 D228 A234 R238 L242 P288 S289 A293 G296 R301 P337 N338

L344 L354 G355 A356 V373 A393 T400 F401 A402 P403 W442 L443 S448 P458 S480 Q511

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain F: 91% 9%

GLY HIS MET SER T3 L4 L5 P9 Q10 Y11 N28 T39 R51 T63 R68 W71 A75 V99 V104 Y122 E144 I151 I198 A234 K235 R238 L242 M257 I276 S289 A293 I310 I314 A327 D336

V339 S351 L354 Y369 V373 T398 Q399 T400 F401 K411 I431 L443 P458 I464 S480 F510 Q511

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain G: % 90% 8%

GLY HIS MET SER T3 L4 L5 P9 Q10 Y11 L17 I49 R68 K81 R94 V99 E114 Y122 I125 C126 V130 I140 W154 W189 S199 R238 I276 S289 A293 T297 R301 A327 V331 Y341 Y369

F401 A402 P403 S428 I431 F432 D435 I439 L443 I452 V453 N454 V455 N456 I457 P458 A462 S480 R491 N497 L502 A505 Q506 G507 I508 K509 PHE GLN

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain H: 88% 11%

GLY HIS MET SER T3 Q10 Y11 L17 G18 E22 N23 E24 R53 R68 W71 A75 V99 C126 A129 V130 I140 L141 P142 I182 W189 K190 G191 S199 K204 K208 D228 R238 N272 D280 L291 V295 Y326

L344 L354 T366 V373 P383 T398 Q399 T400 P403 V423 K424 K434 I439 W442 S448 N454 V455 N456 I457 G469 G470 E471 R478 E479 S480 T495 I496 N497 L504 Q511

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.36Å 159.11Å 157.72Å 90.00° 95.22° 90.00°	Depositor
Resolution (Å)	49.06 – 2.06 49.06 – 2.06	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.06-2.06) 98.3 (49.06-2.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.246 0.185 , 0.242	Depositor DCC
R_{free} test set	11702 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.6	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32399	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5420e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/3937	0.58	0/5343
1	B	0.41	0/3949	0.57	0/5356
1	C	0.43	0/3953	0.58	0/5361
1	D	0.38	0/3901	0.55	0/5300
1	E	0.41	0/3946	0.57	0/5354
1	F	0.41	0/3940	0.58	0/5343
1	G	0.41	0/3898	0.56	0/5292
1	H	0.40	0/3917	0.56	0/5319
All	All	0.41	0/31441	0.57	0/42668

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	3858	0	3839	25	0
1	B	3867	0	3873	30	0
1	C	3868	0	3870	40	0
1	D	3822	0	3785	32	0
1	E	3864	0	3849	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3863	0	3862	25	0
1	G	3820	0	3797	30	0
1	H	3839	0	3809	31	0
2	A	4	0	6	2	0
2	B	4	0	6	0	0
2	F	8	0	12	0	0
3	A	27	0	11	1	0
3	B	54	0	22	3	0
3	C	54	0	22	3	0
3	D	54	0	22	0	0
3	E	27	0	11	0	0
3	F	54	0	22	0	0
3	G	27	0	11	0	0
3	H	27	0	11	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	200	0	0	0	0
5	B	136	0	0	1	0
5	C	153	0	0	1	0
5	D	125	0	0	0	0
5	E	173	0	0	1	0
5	F	162	0	0	0	0
5	G	140	0	0	1	0
5	H	161	0	0	0	0
All	All	32399	0	30840	218	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 4.

All (218) 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:H:272:ASN:HD22	1:H:423:VAL:HG21	1.41	0.82
1:F:151:ILE:HB	1:G:140:ILE:HD11	1.66	0.78
1:F:336:ASP:O	1:F:339:VAL:HG12	1.88	0.73
1:B:331:VAL:HG22	1:B:341:TYR:HD2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HG22	1:B:341:TYR:H	1.61	0.65
1:G:331:VAL:HG22	1:G:341:TYR:CD2	2.34	0.62
1:G:331:VAL:HG22	1:G:341:TYR:HD2	1.65	0.61
1:C:283:LEU:O	1:C:287:VAL:HG12	2.01	0.60
1:B:331:VAL:HG22	1:B:341:TYR:CD2	2.36	0.60
1:G:341:TYR:OH	1:G:403:PRO:HG3	2.01	0.60
1:E:140:ILE:HG13	1:E:151:ILE:HG22	1.84	0.60
1:D:289:SER:HB3	1:D:458:PRO:HG3	1.84	0.60
1:H:68:ARG:HD2	1:H:238:ARG:HB3	1.84	0.60
1:D:18:GLY:O	1:D:204:LYS:NZ	2.33	0.59
1:B:36:GLU:OE2	1:E:393:ALA:HA	2.02	0.59
1:C:331:VAL:HG22	1:C:341:TYR:HD2	1.68	0.59
1:F:289:SER:HB3	1:F:458:PRO:HD3	1.84	0.59
1:C:424:LYS:HE2	1:C:424:LYS:HA	1.83	0.59
1:C:68:ARG:HD2	1:C:238:ARG:HB3	1.85	0.58
1:C:331:VAL:HG22	1:C:341:TYR:CD2	2.38	0.58
1:B:18:GLY:O	1:B:204:LYS:HE2	2.05	0.56
1:C:287:VAL:HG13	1:C:288:PRO:HD3	1.87	0.56
1:E:68:ARG:HD2	1:E:238:ARG:HB3	1.87	0.56
1:F:293:ALA:HB2	1:F:458:PRO:HB2	1.85	0.56
1:G:293:ALA:HB2	1:G:458:PRO:HB2	1.87	0.56
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.88	0.56
1:D:354:LEU:HD21	1:D:373:VAL:HG23	1.87	0.55
1:D:28:ASN:HB3	1:D:63:THR:HG23	1.87	0.55
1:D:20:ARG:NH2	1:D:24:GLU:OE2	2.40	0.55
1:C:443:LEU:HD13	1:D:151:ILE:HD11	1.89	0.54
1:E:442:TRP:CH2	1:E:448:SER:HB2	2.43	0.54
1:F:104:VAL:HA	1:F:198:ILE:HD11	1.89	0.54
1:A:310:ILE:HG22	1:A:314:ILE:HG13	1.90	0.54
1:B:336:ASP:O	1:B:339:VAL:HG12	2.08	0.54
1:E:228:ASP:HB2	5:E:855:HOH:O	2.07	0.54
1:B:372:LYS:NZ	1:B:382:GLU:OE1	2.36	0.54
1:C:287:VAL:HG11	4:C:602:CL:CL	2.45	0.53
1:G:68:ARG:HD2	1:G:238:ARG:HB3	1.90	0.53
1:E:8:GLN:NE2	1:E:10:GLN:OE1	2.41	0.53
1:H:272:ASN:ND2	1:H:423:VAL:HG21	2.20	0.53
1:E:104:VAL:HA	1:E:198:ILE:HD11	1.90	0.52
1:D:293:ALA:HB2	1:D:458:PRO:HB3	1.91	0.52
1:H:280:ASP:O	1:H:434:LYS:HE2	2.09	0.52
1:A:118:GLU:HG3	1:A:171:ALA:HB2	1.91	0.52
1:A:503:PRO:HD3	1:B:285:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ALA:HB2	1:B:458:PRO:HB2	1.90	0.52
1:C:37:VAL:HG22	1:C:53:ARG:HG2	1.92	0.52
1:G:297:THR:OG1	1:G:301:ARG:NE	2.42	0.52
1:H:454:ASN:HB3	1:H:457:ILE:HG13	1.92	0.52
1:H:22:GLU:HG2	1:H:53:ARG:HE	1.75	0.52
1:C:21:GLU:OE2	1:C:51:ARG:NH2	2.41	0.51
1:B:140:ILE:HG22	1:C:138:GLY:O	2.10	0.51
1:D:68:ARG:HD2	1:D:238:ARG:HB3	1.92	0.51
1:G:457:ILE:HD11	1:H:495:THR:HB	1.92	0.51
1:H:126:CYS:O	1:H:130:VAL:HG23	2.09	0.51
1:C:442:TRP:CH2	1:C:448:SER:HB2	2.46	0.51
1:D:374:MET:HE2	1:D:382:GLU:HA	1.93	0.50
1:E:337:PRO:O	1:E:338:ASN:HB3	2.12	0.50
1:G:154:TRP:CH2	1:G:491:ARG:HB2	2.47	0.50
1:E:234:ALA:HA	1:E:242:LEU:HD22	1.92	0.50
1:C:496:ILE:HD11	1:D:443:LEU:HD11	1.94	0.50
1:A:354:LEU:HD12	1:F:351:SER:HB2	1.93	0.50
1:B:68:ARG:HD2	1:B:238:ARG:HB3	1.93	0.50
1:B:391:HIS:HA	1:B:408:PHE:CE1	2.46	0.50
1:H:291:LEU:O	1:H:295:VAL:HG22	2.12	0.49
1:H:439:ILE:HG23	1:H:455:VAL:HG21	1.94	0.49
1:C:285:LEU:HD12	1:D:503:PRO:HD3	1.94	0.49
1:E:151:ILE:HD11	1:F:443:LEU:HD13	1.94	0.49
1:G:293:ALA:HB2	1:G:458:PRO:CB	2.42	0.49
1:H:10:GLN:HG3	1:H:11:TYR:CD2	2.48	0.49
1:A:145:ARG:HH21	1:A:495:THR:HG21	1.78	0.49
1:H:423:VAL:HG22	1:H:424:LYS:H	1.78	0.49
1:E:443:LEU:HD12	1:F:151:ILE:HD11	1.94	0.49
1:A:454:ASN:HB3	1:A:457:ILE:HG23	1.95	0.48
1:C:145:ARG:NH2	1:D:461:GLY:O	2.46	0.48
1:A:331:VAL:HG22	1:A:341:TYR:HD2	1.78	0.48
1:F:68:ARG:HD2	1:F:238:ARG:HB3	1.95	0.48
1:H:190:LYS:NZ	1:H:191:GLY:O	2.42	0.48
1:C:4:LEU:HD23	1:C:48:PRO:HB2	1.96	0.48
1:C:126:CYS:O	1:C:130:VAL:HG23	2.13	0.48
1:C:188:LEU:HD21	1:C:223:THR:HG23	1.96	0.47
1:G:443:LEU:HD11	1:H:496:ILE:HD11	1.95	0.47
1:C:454:ASN:HB3	1:C:457:ILE:HG23	1.96	0.47
1:C:503:PRO:HG2	1:D:288:PRO:HB2	1.97	0.47
1:D:454:ASN:HB3	1:D:457:ILE:HG13	1.96	0.47
1:C:312:GLU:HG3	1:C:410:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:VAL:HG22	1:D:341:TYR:CD2	2.50	0.47
1:C:22:GLU:OE2	1:C:53:ARG:NE	2.46	0.47
1:E:4:LEU:HD23	1:E:48:PRO:HB2	1.96	0.47
1:H:354:LEU:HD21	1:H:373:VAL:HG23	1.96	0.47
1:C:287:VAL:HG13	1:C:288:PRO:CD	2.44	0.46
1:B:454:ASN:HB3	1:B:457:ILE:HG22	1.98	0.46
1:E:293:ALA:HB2	1:E:458:PRO:HB2	1.96	0.46
1:A:331:VAL:HG22	1:A:341:TYR:CD2	2.50	0.46
1:D:331:VAL:HG22	1:D:341:TYR:HD2	1.81	0.46
1:D:296:GLY:HA3	1:D:301:ARG:NH1	2.31	0.46
1:F:354:LEU:HD21	1:F:373:VAL:HG23	1.97	0.46
1:G:435:ASP:O	1:G:439:ILE:HG12	2.16	0.45
1:H:469:GLY:HA3	1:H:478:ARG:HD3	1.96	0.45
1:A:154:TRP:CH2	1:A:491:ARG:HB2	2.51	0.45
1:E:126:CYS:O	1:E:130:VAL:HG23	2.15	0.45
1:E:289:SER:HB3	1:E:458:PRO:HD3	1.98	0.45
1:G:17:LEU:HD21	1:G:99:VAL:HG23	1.97	0.45
1:C:310:ILE:HG22	1:C:314:ILE:HG13	1.99	0.45
1:D:5:LEU:HB2	1:D:49:ILE:HA	1.98	0.45
1:B:97:ILE:HG12	1:B:116:VAL:HG13	1.97	0.45
1:B:276:ILE:HB	1:B:431:ILE:HG22	1.97	0.45
1:E:293:ALA:HB2	1:E:458:PRO:CB	2.47	0.45
1:A:276:ILE:HB	1:A:431:ILE:HG22	1.99	0.45
1:F:151:ILE:HB	1:G:140:ILE:CD1	2.43	0.45
1:H:344:LEU:HD21	1:H:403:PRO:HD3	1.98	0.45
1:A:28:ASN:HD21	2:A:601:EDO:H11	1.81	0.45
1:C:10:GLN:HG3	1:C:11:TYR:CD2	2.52	0.45
1:C:289:SER:HB3	1:C:458:PRO:HD3	1.99	0.45
1:F:327:ALA:HA	1:F:369:TYR:OH	2.16	0.45
1:G:454:ASN:HB3	1:G:457:ILE:HG13	1.99	0.45
1:B:310:ILE:HG22	1:B:314:ILE:HG13	2.00	0.44
1:G:457:ILE:HG23	1:H:497:ASN:HB2	1.98	0.44
1:F:310:ILE:HG22	1:F:314:ILE:HG13	1.98	0.44
1:A:354:LEU:HD21	1:A:373:VAL:HG23	2.00	0.44
1:G:94:ARG:NH1	5:G:704:HOH:O	2.49	0.44
1:D:276:ILE:HB	1:D:431:ILE:HG22	2.00	0.44
1:F:235:LYS:NZ	1:F:257:MET:SD	2.88	0.44
1:B:331:VAL:HG11	1:B:374:MET:SD	2.58	0.44
1:E:4:LEU:HD11	1:E:51:ARG:NH1	2.33	0.44
1:C:324:LYS:HE2	1:C:324:LYS:HB3	1.84	0.44
1:E:4:LEU:HD12	1:E:21:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:CYS:O	1:G:130:VAL:HG23	2.17	0.44
1:H:326:TYR:CE2	1:H:383:PRO:HB2	2.53	0.44
1:H:471:GLU:OE2	1:H:478:ARG:NH2	2.44	0.44
1:A:138:GLY:O	1:D:140:ILE:HG22	2.17	0.44
1:B:142:PRO:HB2	1:C:79:ALA:HB3	1.99	0.43
3:C:601[B]:NAD:H8A	3:C:601[B]:NAD:H2B	1.82	0.43
1:G:497:ASN:HB2	1:H:457:ILE:HG23	1.99	0.43
1:H:71:TRP:CE2	1:H:75:ALA:HB2	2.53	0.43
1:D:175:TRP:HE1	1:D:464:ILE:HD11	1.82	0.43
1:G:428:SER:HA	1:G:452:ILE:HB	2.00	0.43
3:C:601[A]:NAD:H2B	3:C:601[A]:NAD:H8A	1.83	0.43
1:D:145:ARG:HD2	1:D:148:HIS:CD2	2.53	0.43
1:A:419:TRP:O	1:A:422:GLU:HG2	2.18	0.43
1:A:443:LEU:HD11	1:B:496:ILE:HD11	2.00	0.43
1:F:28:ASN:HB3	1:F:63:THR:HG23	2.00	0.43
1:A:442:TRP:CH2	1:A:448:SER:HB2	2.53	0.43
1:A:79:ALA:HB3	1:D:142:PRO:HB2	1.99	0.43
1:E:39:THR:OG1	1:E:51:ARG:HG2	2.19	0.43
1:B:228:ASP:HB2	5:B:798:HOH:O	2.19	0.43
1:D:293:ALA:HB2	1:D:458:PRO:CB	2.49	0.43
3:B:602[B]:NAD:O5D	3:B:602[B]:NAD:H8A	2.18	0.43
1:G:10:GLN:HG3	1:G:11:TYR:CD1	2.53	0.43
1:B:81:LYS:HE2	1:C:144:GLU:O	2.17	0.43
1:C:469:GLY:HA3	1:C:478:ARG:HD3	2.00	0.43
1:G:189:TRP:CH2	1:G:199:SER:HA	2.53	0.43
1:B:341:TYR:OH	1:B:403:PRO:HG3	2.19	0.42
1:C:293:ALA:HB2	1:C:458:PRO:HB2	2.01	0.42
1:G:276:ILE:HB	1:G:431:ILE:HG22	2.01	0.42
1:D:232:ALA:O	1:D:236:ASP:HB2	2.20	0.42
1:G:122:TYR:HA	1:G:125:ILE:HG22	2.02	0.42
1:F:234:ALA:HA	1:F:242:LEU:HD22	2.01	0.42
1:H:22:GLU:OE2	1:H:53:ARG:NE	2.53	0.42
1:B:439:ILE:HG23	1:B:455:VAL:HG21	2.01	0.42
1:D:442:TRP:CH2	1:D:448:SER:HB2	2.54	0.42
1:E:10:GLN:H	1:E:10:GLN:HG3	1.35	0.42
1:F:71:TRP:CE2	1:F:75:ALA:HB2	2.54	0.42
1:C:105:SER:OG	1:C:112:LEU:HA	2.19	0.42
1:E:138:GLY:O	1:H:140:ILE:HG22	2.19	0.42
1:G:5:LEU:HB2	1:G:49:ILE:HA	2.01	0.42
1:B:327:ALA:HA	1:B:369:TYR:OH	2.19	0.42
1:B:331:VAL:HG21	1:B:374:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:SER:HB3	1:B:458:PRO:HD3	2.02	0.42
1:C:246:GLY:HA3	3:C:601[A]:NAD:H51A	2.01	0.42
1:F:5:LEU:O	1:F:11:TYR:HB2	2.20	0.42
1:C:341:TYR:OH	1:C:403:PRO:HG3	2.20	0.42
1:D:469:GLY:HA3	1:D:478:ARG:HD3	2.02	0.42
1:E:354:LEU:HD21	1:E:373:VAL:HG23	2.02	0.42
1:E:5:LEU:HD22	1:E:11:TYR:CE2	2.54	0.42
1:E:443:LEU:CD1	1:F:151:ILE:HD11	2.49	0.42
1:A:472:LYS:HE3	1:A:472:LYS:HB2	1.82	0.42
1:B:344:LEU:HD21	1:B:403:PRO:HD3	2.02	0.42
1:C:506:GLN:O	1:D:330:ARG:NH2	2.49	0.42
1:C:99:VAL:HG22	5:C:811:HOH:O	2.19	0.41
1:E:136:ILE:O	1:H:142:PRO:HD3	2.20	0.41
1:G:432:PHE:CD2	1:G:456:ASN:HA	2.55	0.41
1:E:344:LEU:HD21	1:E:403:PRO:HD3	2.03	0.41
1:A:5:LEU:HB2	1:A:49:ILE:HA	2.02	0.41
1:E:296:GLY:HA3	1:E:301:ARG:NH1	2.36	0.41
1:F:144:GLU:O	1:G:81:LYS:HE3	2.19	0.41
1:H:129:ALA:HB1	1:H:182:ILE:HG21	2.02	0.41
1:H:442:TRP:CH2	1:H:448:SER:HB2	2.56	0.41
1:A:28:ASN:HD21	2:A:601:EDO:H21	1.86	0.41
1:F:276:ILE:HB	1:F:431:ILE:HG22	2.02	0.41
1:C:494:CYS:HA	1:D:453:VAL:O	2.20	0.41
3:B:602[B]:NAD:H2B	3:B:602[B]:NAD:H8A	1.92	0.41
1:D:341:TYR:OH	1:D:403:PRO:HG3	2.20	0.41
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.91	0.41
1:D:323:LYS:HD2	1:D:368:VAL:HG22	2.03	0.41
1:C:234:ALA:HA	1:C:242:LEU:HD22	2.03	0.41
1:H:189:TRP:CH2	1:H:199:SER:HA	2.56	0.41
1:E:356:ALA:HB2	1:E:400:THR:HG21	2.03	0.41
1:F:39:THR:OG1	1:F:51:ARG:HG2	2.20	0.41
1:F:464:ILE:HA	1:F:464:ILE:HD13	1.84	0.41
1:H:423:VAL:HG22	1:H:424:LYS:N	2.35	0.41
1:A:372:LYS:HB2	1:A:372:LYS:HE2	1.93	0.40
1:B:138:GLY:O	1:C:140:ILE:HG22	2.21	0.40
1:H:17:LEU:HD21	1:H:99:VAL:HG23	2.03	0.40
3:B:602[A]:NAD:H8A	3:B:602[A]:NAD:H2B	1.93	0.40
1:C:376:ARG:HB2	1:C:377:PRO:HD2	2.03	0.40
1:D:391:HIS:HA	1:D:408:PHE:CE1	2.56	0.40
1:E:442:TRP:CZ2	1:E:448:SER:HB2	2.56	0.40
1:E:288:PRO:HB3	1:F:510:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:GLU:OE2	1:G:301:ARG:NH1	2.51	0.40
1:G:327:ALA:HA	1:G:369:TYR:OH	2.22	0.40
1:G:289:SER:HB3	1:G:458:PRO:HD3	2.03	0.40
1:A:246:GLY:HA3	3:A:602:NAD:H51A	2.04	0.40
1:B:154:TRP:CH2	1:B:491:ARG:HB2	2.56	0.40
1:F:411:LYS:HB2	1:F:411:LYS:HE2	1.72	0.40
1:A:182:ILE:HG13	1:A:183:CYS:N	2.37	0.40
1:A:374:MET:HE2	1:A:382:GLU:HA	2.03	0.40
1:H:18:GLY:O	1:H:204:LYS:HE3	2.21	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	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	39
1	B	508/513 (99%)	491 (97%)	16 (3%)	1 (0%)	47	39
1	C	509/513 (99%)	491 (96%)	17 (3%)	1 (0%)	47	39
1	D	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	47	39
1	E	508/513 (99%)	490 (96%)	17 (3%)	1 (0%)	47	39
1	F	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	47	39
1	G	505/513 (98%)	489 (97%)	15 (3%)	1 (0%)	47	39
1	H	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	39
All	All	4058/4104 (99%)	3925 (97%)	125 (3%)	8 (0%)	47	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER

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

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	401/410 (98%)	394 (98%)	7 (2%)	60	57
1	B	403/410 (98%)	397 (98%)	6 (2%)	65	62
1	C	403/410 (98%)	394 (98%)	9 (2%)	52	46
1	D	392/410 (96%)	385 (98%)	7 (2%)	59	55
1	E	403/410 (98%)	398 (99%)	5 (1%)	71	69
1	F	404/410 (98%)	397 (98%)	7 (2%)	60	57
1	G	394/410 (96%)	392 (100%)	2 (0%)	88	89
1	H	396/410 (97%)	388 (98%)	8 (2%)	55	51
All	All	3196/3280 (97%)	3145 (98%)	51 (2%)	62	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	122	TYR
1	A	208	LYS
1	A	297	THR
1	A	398	THR
1	A	400	THR
1	A	509	LYS
1	B	113	VAL

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Mol	Chain	Res	Type
1	B	340	LEU
1	B	394	SER
1	B	398	THR
1	B	401	PHE
1	B	443	LEU
1	C	24	GLU
1	C	188	LEU
1	C	287	VAL
1	C	297	THR
1	C	324	LYS
1	C	340	LEU
1	C	348	GLN
1	C	354	LEU
1	C	400	THR
1	D	10	GLN
1	D	99	VAL
1	D	352	MET
1	D	362	LYS
1	D	398	THR
1	D	430	SER
1	D	504	LEU
1	E	10	GLN
1	E	122	TYR
1	E	400	THR
1	E	401	PHE
1	E	443	LEU
1	F	3	THR
1	F	99	VAL
1	F	122	TYR
1	F	398	THR
1	F	400	THR
1	F	401	PHE
1	F	511	GLN
1	G	297	THR
1	G	401	PHE
1	H	24	GLU
1	H	208	LYS
1	H	228	ASP
1	H	291	LEU
1	H	366	THR
1	H	398	THR
1	H	400	THR

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Mol	Chain	Res	Type
1	H	504	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	B	10	GLN
1	B	473	HIS
1	D	338	ASN
1	D	506	GLN
1	E	7	ASN
1	F	249	GLN
1	G	399	GLN
1	H	10	GLN
1	H	272	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 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
3	NAD	B	602[A]	-	24,29,48	4.85	9 (37%)	29,45,73	1.52	3 (10%)
2	EDO	B	601	-	3,3,3	0.48	0	2,2,2	0.31	0
3	NAD	F	603[B]	-	24,29,48	4.86	8 (33%)	29,45,73	1.46	3 (10%)
3	NAD	B	602[B]	-	24,29,48	4.82	8 (33%)	29,45,73	1.57	5 (17%)
3	NAD	D	601[A]	-	24,29,48	4.93	8 (33%)	29,45,73	1.48	2 (6%)
3	NAD	H	601	-	24,29,48	4.82	8 (33%)	29,45,73	1.41	3 (10%)
3	NAD	A	602	-	24,29,48	4.76	9 (37%)	29,45,73	1.33	3 (10%)
3	NAD	G	601	-	24,29,48	4.81	8 (33%)	29,45,73	1.39	3 (10%)
2	EDO	A	601	-	3,3,3	0.43	0	2,2,2	0.63	0
2	EDO	F	602	-	3,3,3	0.46	0	2,2,2	0.42	0
3	NAD	C	601[B]	-	24,29,48	4.95	9 (37%)	29,45,73	1.48	3 (10%)
3	NAD	D	601[B]	-	24,29,48	4.93	8 (33%)	29,45,73	1.50	3 (10%)
3	NAD	C	601[A]	-	24,29,48	4.92	9 (37%)	29,45,73	1.46	3 (10%)
3	NAD	F	603[A]	-	24,29,48	4.82	8 (33%)	29,45,73	1.43	2 (6%)
3	NAD	E	601	-	24,29,48	4.89	7 (29%)	29,45,73	1.59	6 (20%)
2	EDO	F	601	-	3,3,3	0.50	0	2,2,2	0.28	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
3	NAD	B	602[A]	-	-	7/12/32/62	0/3/3/5
2	EDO	B	601	-	-	1/1/1/1	-
3	NAD	F	603[B]	-	-	2/12/32/62	0/3/3/5
3	NAD	B	602[B]	-	-	4/12/32/62	0/3/3/5
3	NAD	D	601[A]	-	-	1/12/32/62	0/3/3/5
3	NAD	H	601	-	-	3/12/32/62	0/3/3/5
3	NAD	A	602	-	-	3/12/32/62	0/3/3/5
3	NAD	G	601	-	-	4/12/32/62	0/3/3/5
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	F	602	-	-	0/1/1/1	-
3	NAD	C	601[B]	-	-	2/12/32/62	0/3/3/5
3	NAD	D	601[B]	-	-	3/12/32/62	0/3/3/5
3	NAD	C	601[A]	-	-	5/12/32/62	0/3/3/5
3	NAD	F	603[A]	-	-	3/12/32/62	0/3/3/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	E	601	-	-	1/12/32/62	0/3/3/5
2	EDO	F	601	-	-	0/1/1/1	-

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	601	NAD	C2B-C1B	-16.32	1.29	1.53
3	D	601[B]	NAD	C2B-C1B	-16.13	1.29	1.53
3	C	601[B]	NAD	C2B-C1B	-16.11	1.29	1.53
3	D	601[A]	NAD	C2B-C1B	-16.10	1.29	1.53
3	G	601	NAD	C2B-C1B	-16.08	1.29	1.53
3	E	601	NAD	C2B-C1B	-16.02	1.29	1.53
3	C	601[A]	NAD	C2B-C1B	-16.01	1.29	1.53
3	F	603[B]	NAD	C2B-C1B	-15.98	1.29	1.53
3	F	603[A]	NAD	C2B-C1B	-15.89	1.29	1.53
3	B	602[A]	NAD	C2B-C1B	-15.74	1.29	1.53
3	A	602	NAD	C2B-C1B	-15.63	1.30	1.53
3	B	602[B]	NAD	O4B-C1B	15.28	1.62	1.41
3	D	601[B]	NAD	O4B-C1B	15.27	1.62	1.41
3	D	601[A]	NAD	O4B-C1B	15.25	1.62	1.41
3	C	601[B]	NAD	O4B-C1B	15.25	1.62	1.41
3	B	602[B]	NAD	C2B-C1B	-15.24	1.30	1.53
3	C	601[A]	NAD	O4B-C1B	15.09	1.62	1.41
3	E	601	NAD	O4B-C1B	15.07	1.62	1.41
3	B	602[A]	NAD	O4B-C1B	15.01	1.62	1.41
3	F	603[B]	NAD	O4B-C1B	14.96	1.61	1.41
3	F	603[A]	NAD	O4B-C1B	14.82	1.61	1.41
3	G	601	NAD	O4B-C1B	14.35	1.61	1.41
3	H	601	NAD	O4B-C1B	14.34	1.61	1.41
3	A	602	NAD	O4B-C1B	14.13	1.60	1.41
3	G	601	NAD	O4B-C4B	-6.30	1.30	1.45
3	A	602	NAD	O4B-C4B	-6.29	1.30	1.45
3	F	603[B]	NAD	O4B-C4B	-6.29	1.30	1.45
3	D	601[A]	NAD	O4B-C4B	-6.27	1.31	1.45
3	D	601[B]	NAD	O4B-C4B	-6.24	1.31	1.45
3	F	603[A]	NAD	O4B-C4B	-6.18	1.31	1.45
3	C	601[B]	NAD	O4B-C4B	-6.15	1.31	1.45
3	C	601[A]	NAD	O4B-C4B	-6.09	1.31	1.45
3	E	601	NAD	O4B-C4B	-6.08	1.31	1.45
3	B	602[A]	NAD	O4B-C4B	-5.87	1.31	1.45
3	H	601	NAD	O4B-C4B	-5.80	1.32	1.45
3	B	602[B]	NAD	O4B-C4B	-5.72	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601[A]	NAD	C2A-N3A	3.37	1.37	1.32
3	C	601[B]	NAD	C2A-N3A	3.26	1.37	1.32
3	D	601[A]	NAD	O3B-C3B	-3.25	1.35	1.43
3	E	601	NAD	O2B-C2B	3.23	1.50	1.43
3	E	601	NAD	O3B-C3B	-3.22	1.35	1.43
3	A	602	NAD	O2B-C2B	3.21	1.50	1.43
3	D	601[B]	NAD	O3B-C3B	-3.20	1.35	1.43
3	A	602	NAD	C2A-N3A	3.17	1.37	1.32
3	G	601	NAD	O2B-C2B	3.10	1.50	1.43
3	F	603[B]	NAD	O3B-C3B	-3.04	1.35	1.43
3	G	601	NAD	O3B-C3B	-3.03	1.35	1.43
3	B	602[B]	NAD	C2A-N3A	3.02	1.37	1.32
3	A	602	NAD	PN-O1N	3.02	1.60	1.50
3	H	601	NAD	C2A-N3A	3.01	1.36	1.32
3	H	601	NAD	O2B-C2B	3.01	1.50	1.43
3	C	601[A]	NAD	O2B-C2B	3.00	1.50	1.43
3	F	603[A]	NAD	O3B-C3B	-3.00	1.35	1.43
3	C	601[A]	NAD	PN-O1N	2.99	1.60	1.50
3	B	602[A]	NAD	PN-O1N	2.99	1.60	1.50
3	G	601	NAD	C2A-N3A	2.98	1.36	1.32
3	C	601[B]	NAD	O2B-C2B	2.98	1.50	1.43
3	B	602[B]	NAD	O2B-C2B	2.96	1.49	1.43
3	B	602[A]	NAD	C2A-N3A	2.96	1.36	1.32
3	B	602[B]	NAD	PN-O1N	2.94	1.60	1.50
3	C	601[A]	NAD	O3B-C3B	-2.93	1.36	1.43
3	B	602[A]	NAD	O3B-C3B	-2.93	1.36	1.43
3	F	603[B]	NAD	O2B-C2B	2.86	1.49	1.43
3	C	601[B]	NAD	PN-O1N	2.86	1.59	1.50
3	D	601[B]	NAD	C2A-N3A	2.85	1.36	1.32
3	B	602[B]	NAD	O3B-C3B	-2.84	1.36	1.43
3	D	601[A]	NAD	C2A-N3A	2.83	1.36	1.32
3	C	601[B]	NAD	O3B-C3B	-2.81	1.36	1.43
3	B	602[A]	NAD	O2B-C2B	2.77	1.49	1.43
3	D	601[B]	NAD	O2B-C2B	2.77	1.49	1.43
3	D	601[A]	NAD	O2B-C2B	2.77	1.49	1.43
3	A	602	NAD	O3B-C3B	-2.74	1.36	1.43
3	B	602[B]	NAD	C6A-N6A	2.74	1.44	1.34
3	F	603[A]	NAD	O2B-C2B	2.73	1.49	1.43
3	B	602[A]	NAD	C6A-N6A	2.71	1.43	1.34
3	F	603[B]	NAD	C6A-N6A	2.70	1.43	1.34
3	F	603[A]	NAD	C6A-N6A	2.70	1.43	1.34
3	H	601	NAD	C6A-N6A	2.68	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601[A]	NAD	C6A-N6A	2.66	1.43	1.34
3	D	601[B]	NAD	C6A-N6A	2.66	1.43	1.34
3	H	601	NAD	O3B-C3B	-2.62	1.36	1.43
3	F	603[A]	NAD	C2A-N3A	2.61	1.36	1.32
3	F	603[B]	NAD	C2A-N3A	2.59	1.36	1.32
3	E	601	NAD	C6A-N6A	2.57	1.43	1.34
3	C	601[B]	NAD	C6A-N6A	2.54	1.43	1.34
3	C	601[A]	NAD	C6A-N6A	2.53	1.43	1.34
3	A	602	NAD	C6A-N6A	2.50	1.43	1.34
3	G	601	NAD	C6A-N6A	2.40	1.42	1.34
3	G	601	NAD	C5A-C4A	-2.31	1.34	1.40
3	E	601	NAD	C2A-N3A	2.24	1.35	1.32
3	H	601	NAD	C5A-C4A	-2.21	1.35	1.40
3	A	602	NAD	C2A-N1A	2.10	1.37	1.33
3	C	601[B]	NAD	C5A-C4A	-2.09	1.35	1.40
3	D	601[B]	NAD	C5A-C4A	-2.09	1.35	1.40
3	D	601[A]	NAD	C5A-C4A	-2.09	1.35	1.40
3	C	601[A]	NAD	C5A-C4A	-2.06	1.35	1.40
3	B	602[A]	NAD	C5A-C4A	-2.06	1.35	1.40
3	F	603[A]	NAD	C5A-C4A	-2.05	1.35	1.40
3	F	603[B]	NAD	C5A-C4A	-2.01	1.35	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601[B]	NAD	N3A-C2A-N1A	-5.44	120.17	128.68
3	B	602[A]	NAD	N3A-C2A-N1A	-5.43	120.19	128.68
3	D	601[B]	NAD	N3A-C2A-N1A	-5.42	120.20	128.68
3	D	601[A]	NAD	N3A-C2A-N1A	-5.41	120.22	128.68
3	C	601[A]	NAD	N3A-C2A-N1A	-5.39	120.25	128.68
3	G	601	NAD	N3A-C2A-N1A	-5.38	120.26	128.68
3	H	601	NAD	N3A-C2A-N1A	-5.38	120.28	128.68
3	B	602[B]	NAD	N3A-C2A-N1A	-5.31	120.37	128.68
3	F	603[A]	NAD	N3A-C2A-N1A	-5.28	120.43	128.68
3	F	603[B]	NAD	N3A-C2A-N1A	-5.24	120.49	128.68
3	E	601	NAD	N3A-C2A-N1A	-4.84	121.11	128.68
3	A	602	NAD	N3A-C2A-N1A	-4.26	122.02	128.68
3	E	601	NAD	C5A-C6A-N6A	4.06	126.52	120.35
3	B	602[B]	NAD	C5A-C6A-N6A	3.74	126.04	120.35
3	B	602[A]	NAD	C5A-C6A-N6A	3.60	125.82	120.35
3	C	601[B]	NAD	PA-O3-PN	-3.36	121.29	132.83
3	D	601[B]	NAD	C5A-C6A-N6A	3.27	125.32	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601[A]	NAD	C5A-C6A-N6A	3.25	125.29	120.35
3	F	603[B]	NAD	C5A-C6A-N6A	3.23	125.26	120.35
3	F	603[A]	NAD	C5A-C6A-N6A	3.14	125.13	120.35
3	G	601	NAD	C5A-C6A-N6A	2.85	124.69	120.35
3	H	601	NAD	C5A-C6A-N6A	2.79	124.59	120.35
3	A	602	NAD	C5A-C6A-N6A	2.74	124.51	120.35
3	C	601[A]	NAD	C5A-C6A-N6A	2.73	124.50	120.35
3	C	601[B]	NAD	C5A-C6A-N6A	2.67	124.41	120.35
3	E	601	NAD	C1B-N9A-C4A	-2.44	122.35	126.64
3	F	603[B]	NAD	PA-O3-PN	-2.32	124.86	132.83
3	A	602	NAD	O4B-C1B-C2B	-2.29	103.58	106.93
3	B	602[B]	NAD	PA-O3-PN	-2.25	125.12	132.83
3	D	601[B]	NAD	PA-O3-PN	-2.24	125.15	132.83
3	E	601	NAD	N6A-C6A-N1A	-2.21	113.98	118.57
3	G	601	NAD	O5D-PN-O3	2.20	112.02	104.64
3	E	601	NAD	PA-O3-PN	-2.19	125.31	132.83
3	B	602[B]	NAD	O2N-PN-O3	2.16	111.88	104.64
3	E	601	NAD	O5D-PN-O3	2.13	111.79	104.64
3	B	602[B]	NAD	N6A-C6A-N1A	-2.11	114.19	118.57
3	C	601[A]	NAD	PA-O3-PN	-2.06	125.75	132.83
3	B	602[A]	NAD	N6A-C6A-N1A	-2.05	114.33	118.57
3	H	601	NAD	O4B-C1B-C2B	-2.03	103.96	106.93

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAD	C5B-O5B-PA-O1A
3	G	601	NAD	C5B-O5B-PA-O1A
3	G	601	NAD	C5B-O5B-PA-O2A
3	G	601	NAD	PN-O3-PA-O5B
3	B	602[A]	NAD	C5B-O5B-PA-O1A
3	B	602[A]	NAD	C5B-O5B-PA-O2A
3	B	602[A]	NAD	PN-O3-PA-O5B
3	B	602[B]	NAD	PA-O3-PN-O2N
3	D	601[A]	NAD	PN-O3-PA-O5B
3	H	601	NAD	C5B-O5B-PA-O1A
3	H	601	NAD	C5B-O5B-PA-O2A
3	F	603[A]	NAD	PA-O3-PN-O2N
3	F	603[B]	NAD	C5B-O5B-PA-O3
3	C	601[A]	NAD	PA-O3-PN-O2N
2	A	601	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	602[B]	NAD	PA-O3-PN-O1N
3	A	602	NAD	PN-O3-PA-O5B
3	B	602[B]	NAD	PN-O3-PA-O5B
3	D	601[B]	NAD	PN-O3-PA-O5B
3	D	601[B]	NAD	PA-O3-PN-O2N
3	C	601[A]	NAD	PA-O3-PN-O5D
3	C	601[B]	NAD	C5B-O5B-PA-O3
3	F	603[B]	NAD	C5B-O5B-PA-O1A
3	C	601[A]	NAD	C5B-O5B-PA-O1A
3	B	602[A]	NAD	PA-O3-PN-O1N
3	C	601[A]	NAD	PN-O3-PA-O5B
3	F	603[A]	NAD	PA-O3-PN-O5D
3	A	602	NAD	C5B-O5B-PA-O3
3	G	601	NAD	C5B-O5B-PA-O3
3	B	602[A]	NAD	C5B-O5B-PA-O3
3	B	602[B]	NAD	C5B-O5B-PA-O3
3	H	601	NAD	C5B-O5B-PA-O3
3	C	601[A]	NAD	C5B-O5B-PA-O3
3	B	602[A]	NAD	PN-O3-PA-O1A
3	E	601	NAD	C5B-O5B-PA-O1A
3	D	601[B]	NAD	C5B-O5B-PA-O1A
3	C	601[B]	NAD	C5B-O5B-PA-O2A
3	F	603[A]	NAD	C3B-C4B-C5B-O5B
2	B	601	EDO	O1-C1-C2-O2
3	B	602[A]	NAD	C4B-C5B-O5B-PA

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602[A]	NAD	1	0
3	B	602[B]	NAD	2	0
3	A	602	NAD	1	0
2	A	601	EDO	2	0
3	C	601[B]	NAD	1	0
3	C	601[A]	NAD	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 B 602 (A)

Bond lengths　　Bond angles

Torsions　　Rings

Ligand NAD F 603 (B)

Bond lengths　　Bond angles

Torsions　　Rings

Ligand NAD B 602 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 601 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD H 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 601 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 601 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 601 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD F 603 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD E 601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.29	1 (0%)	95	95	20, 29, 45, 75	0
1	B	509/513 (99%)	-0.24	3 (0%)	89	90	22, 33, 53, 71	0
1	C	509/513 (99%)	-0.22	3 (0%)	89	90	20, 32, 54, 82	0
1	D	509/513 (99%)	-0.20	0	100	100	21, 36, 57, 74	0
1	E	509/513 (99%)	-0.36	0	100	100	22, 32, 49, 68	0
1	F	509/513 (99%)	-0.26	1 (0%)	95	95	23, 31, 49, 64	0
1	G	507/513 (98%)	-0.27	6 (1%)	79	80	23, 33, 51, 77	0
1	H	509/513 (99%)	-0.18	0	100	100	22, 34, 57, 78	0
All	All	4070/4104 (99%)	-0.25	14 (0%)	94	94	20, 32, 53, 82	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	502	LEU	3.8
1	G	508	ILE	3.1
1	B	390	GLY	2.9
1	G	507	GLY	2.8
1	C	505	ALA	2.7
1	C	502	LEU	2.4
1	A	9	PRO	2.4
1	B	3	THR	2.4
1	B	335	TRP	2.4
1	G	462	ALA	2.3
1	F	9	PRO	2.2
1	C	503	PRO	2.1
1	G	505	ALA	2.1
1	G	9	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	EDO	F	601	4/4	0.90	0.19	36,47,49,52	0
2	EDO	B	601	4/4	0.92	0.15	37,38,43,44	0
2	EDO	A	601	4/4	0.92	0.22	40,43,43,46	0
3	NAD	A	602	27/44	0.93	0.12	24,37,78,82	0
4	CL	B	603	1/1	0.93	0.07	45,45,45,45	0
3	NAD	E	601	27/44	0.94	0.12	32,39,68,74	0
3	NAD	H	601	27/44	0.94	0.12	33,42,78,81	0
3	NAD	F	603[A]	27/44	0.94	0.12	24,34,41,43	27
3	NAD	F	603[B]	27/44	0.94	0.12	26,34,40,45	27
3	NAD	C	601[B]	27/44	0.94	0.12	27,34,39,44	27
4	CL	D	602	1/1	0.94	0.26	61,61,61,61	0
3	NAD	C	601[A]	27/44	0.94	0.12	30,34,43,47	27
3	NAD	D	601[B]	27/44	0.95	0.12	31,38,50,51	27
3	NAD	B	602[A]	27/44	0.95	0.10	26,30,38,41	27
3	NAD	B	602[B]	27/44	0.95	0.10	24,30,44,47	27
4	CL	E	603	1/1	0.95	0.04	40,40,40,40	0
3	NAD	D	601[A]	27/44	0.95	0.12	31,38,50,51	27
3	NAD	G	601	27/44	0.95	0.10	25,32,72,76	0
4	CL	G	602	1/1	0.95	0.09	50,50,50,50	0
4	CL	C	602	1/1	0.96	0.06	46,46,46,46	0
4	CL	E	602	1/1	0.96	0.04	43,43,43,43	0
2	EDO	F	602	4/4	0.96	0.13	33,35,44,50	0
4	CL	A	603	1/1	0.98	0.07	45,45,45,45	0
4	CL	H	602	1/1	0.99	0.10	54,54,54,54	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 A 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
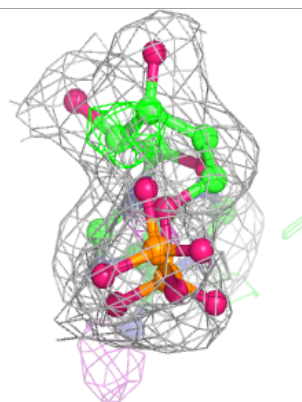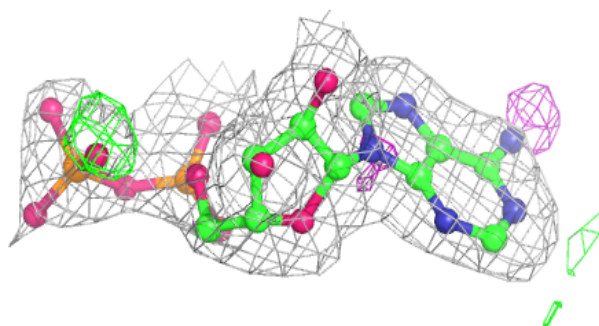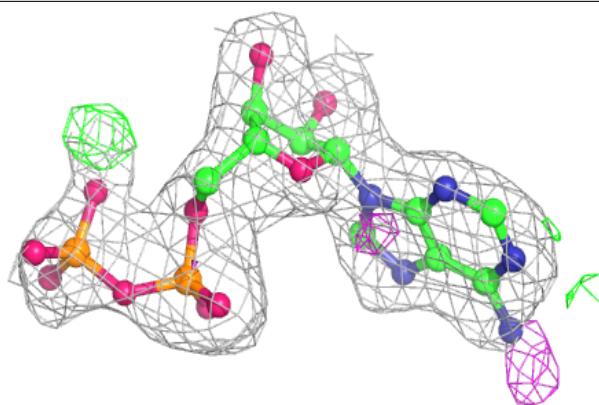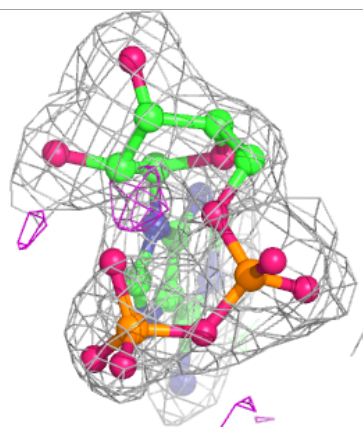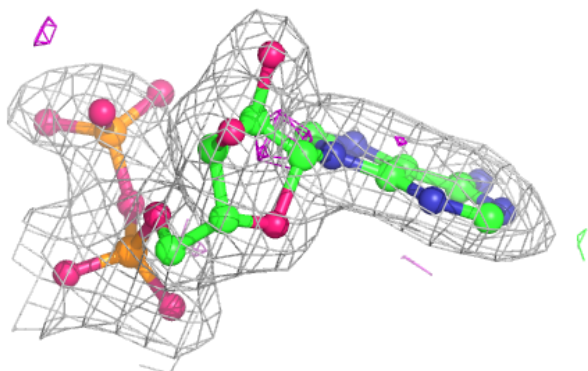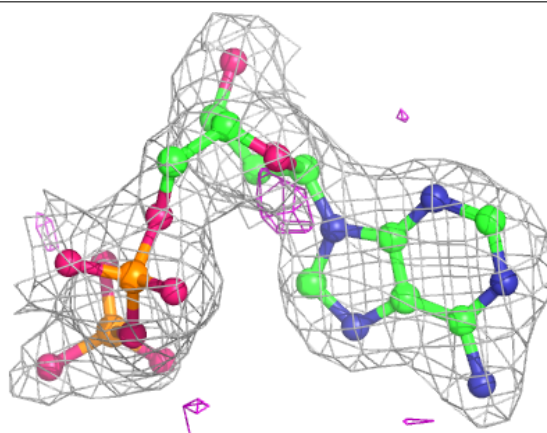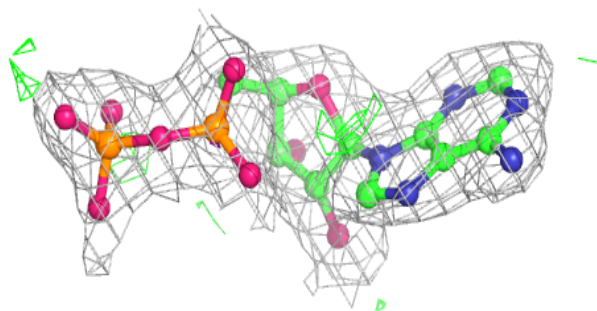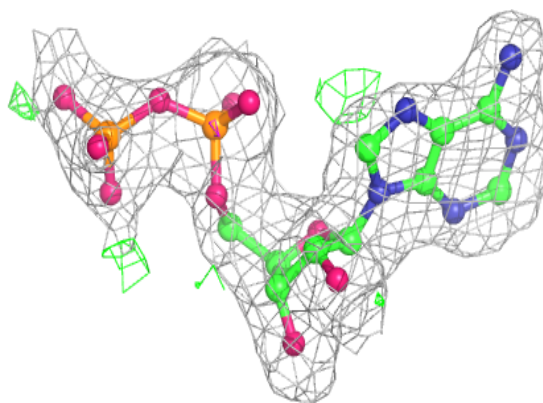and green (positive)
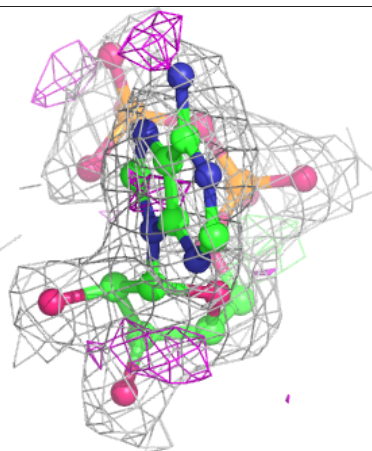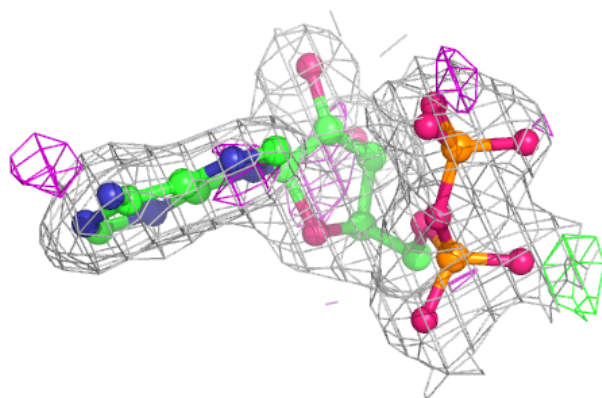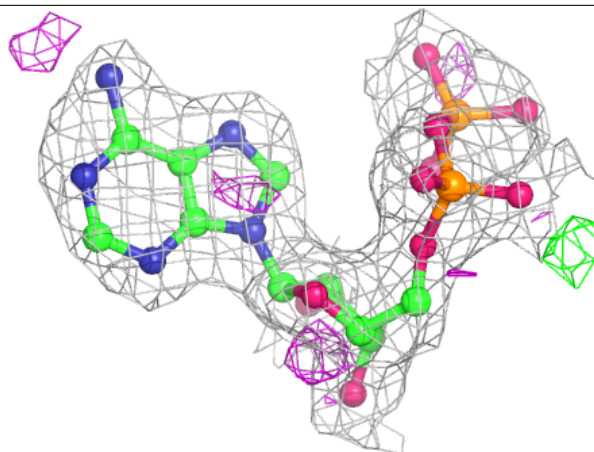
Electron density around NAD E 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
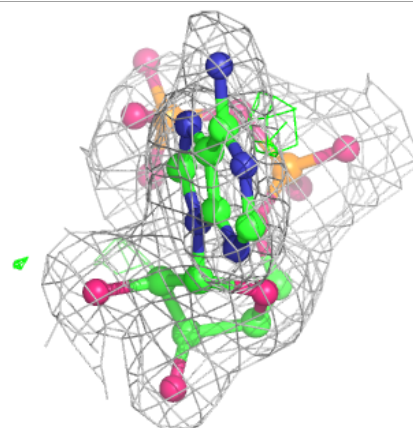mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
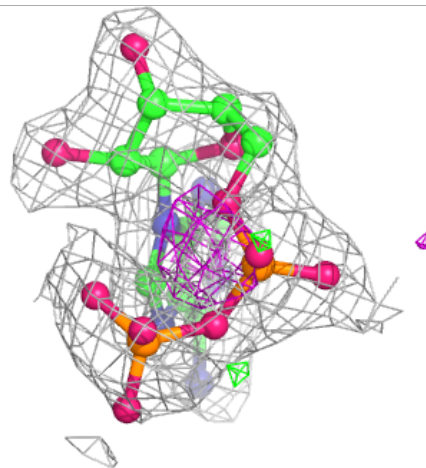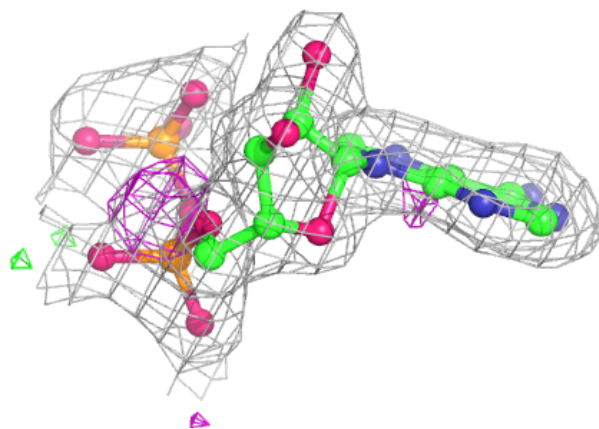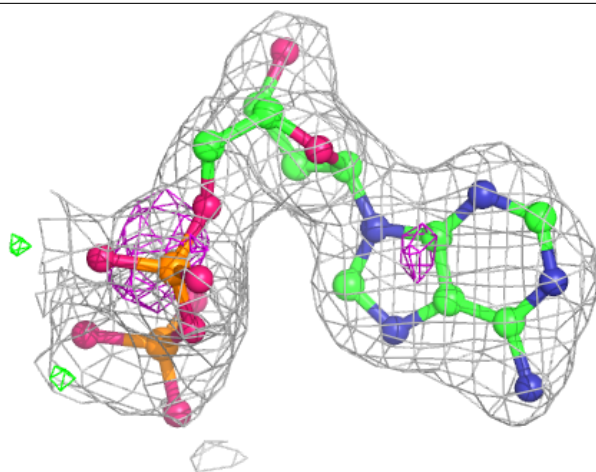
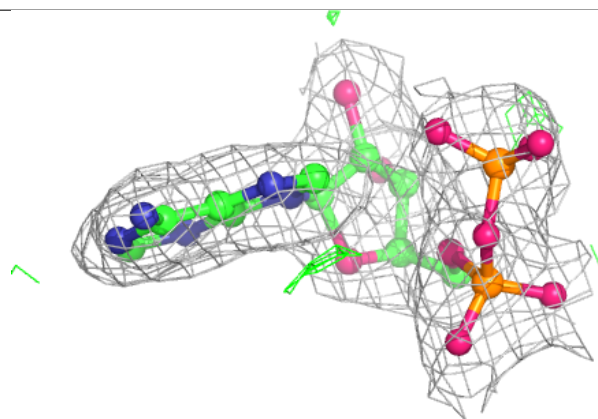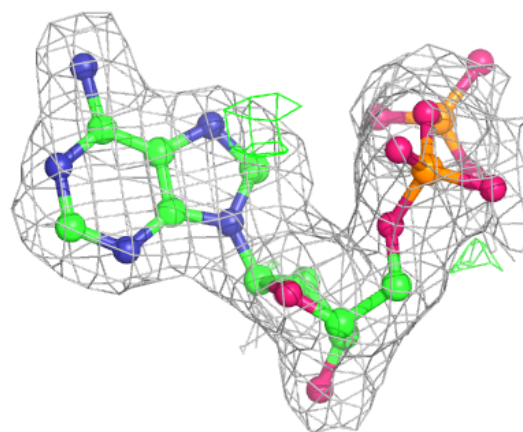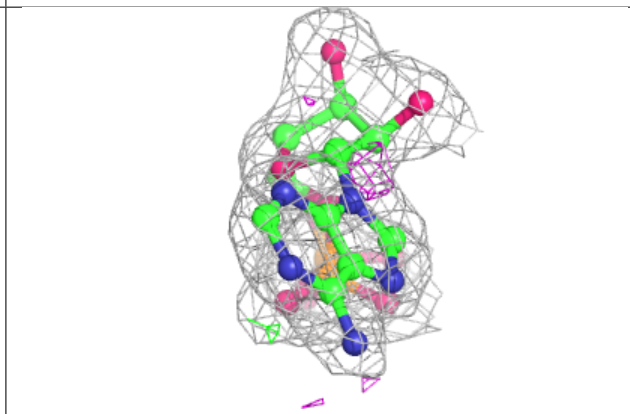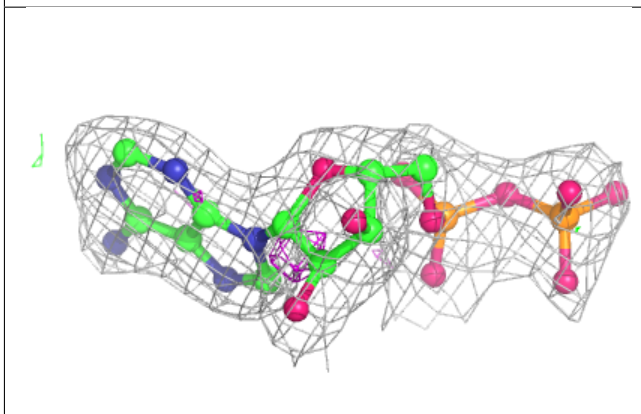**Electron density around NAD H 601:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
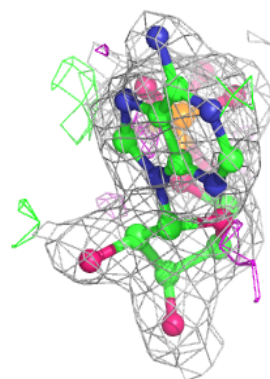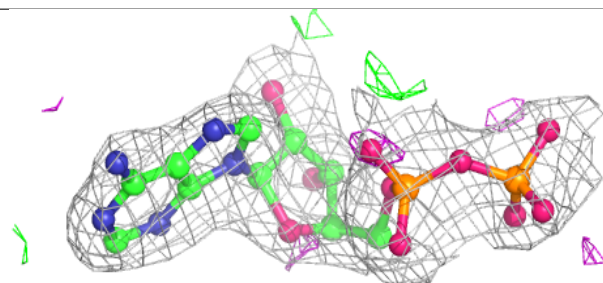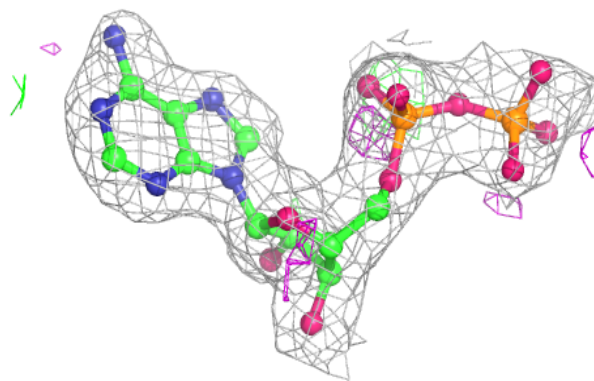
Electron density around NAD F 603 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
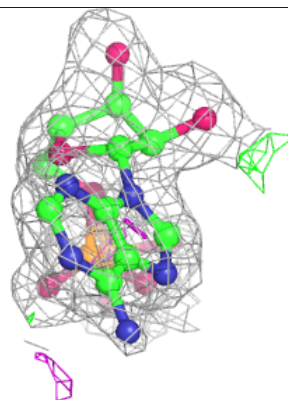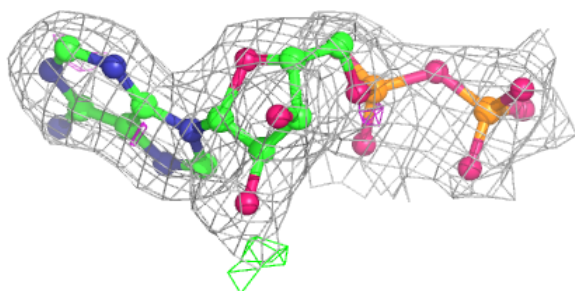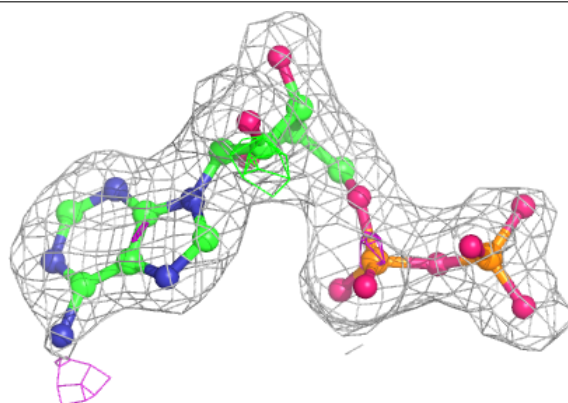
Electron density around NAD F 603 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
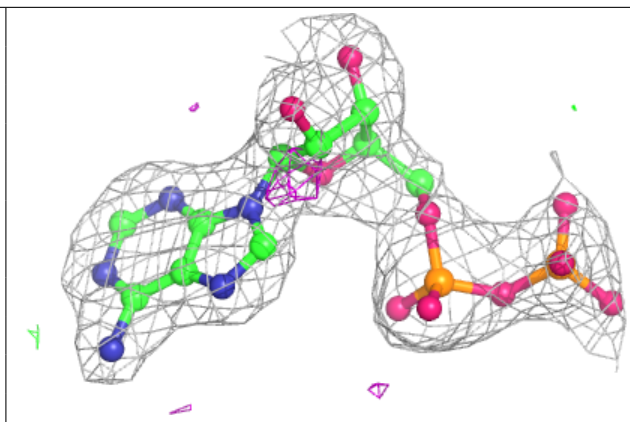and green (positive)
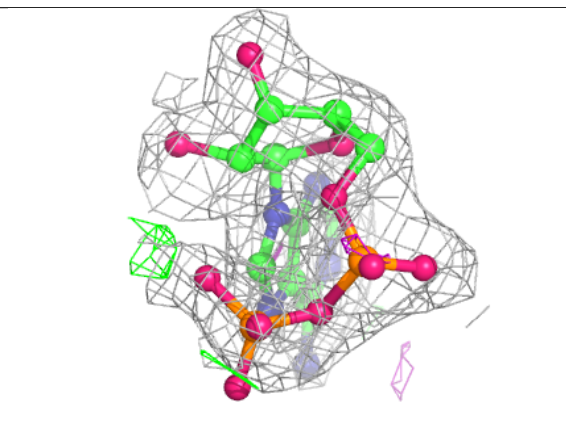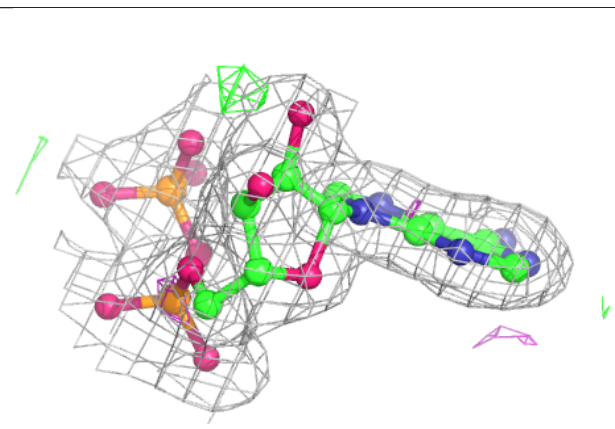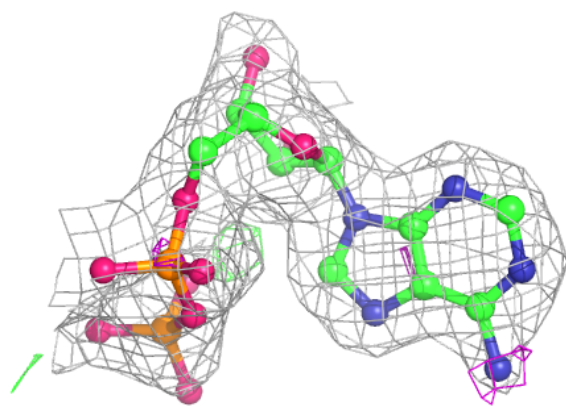
Electron density around NAD C 601 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
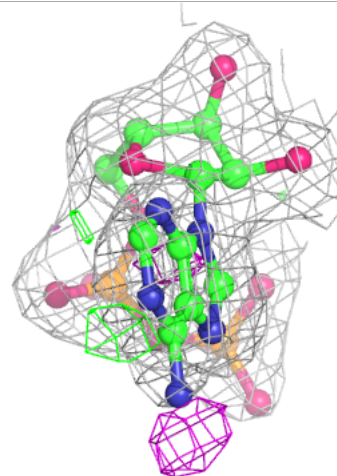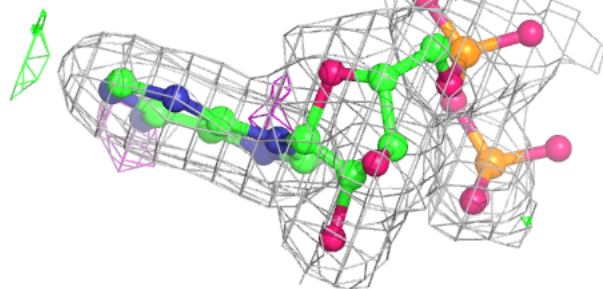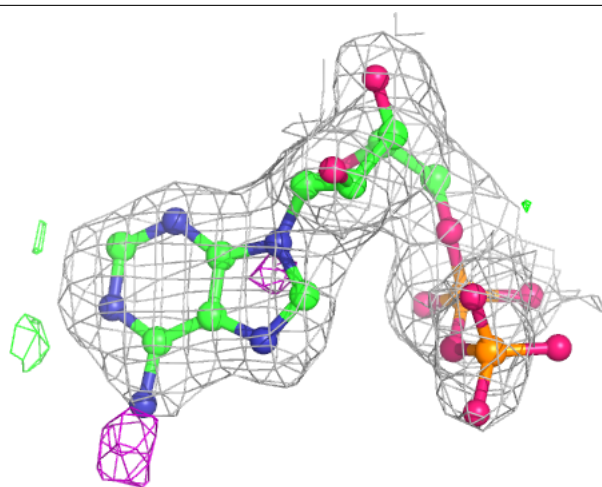
Electron density around NAD C 601 (A):

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

Electron density around NAD D 601 (B):

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

Electron density around NAD B 602 (A):

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

Electron density around NAD B 602 (B):

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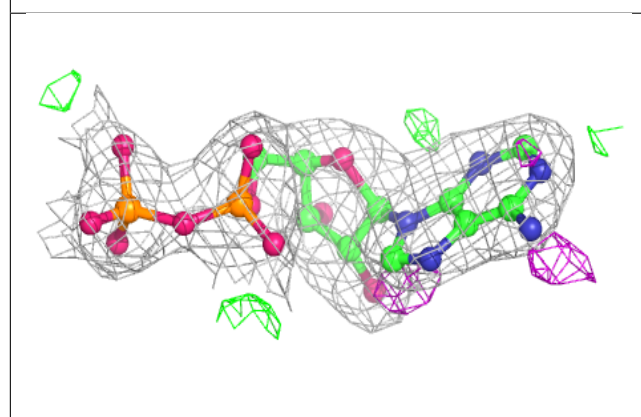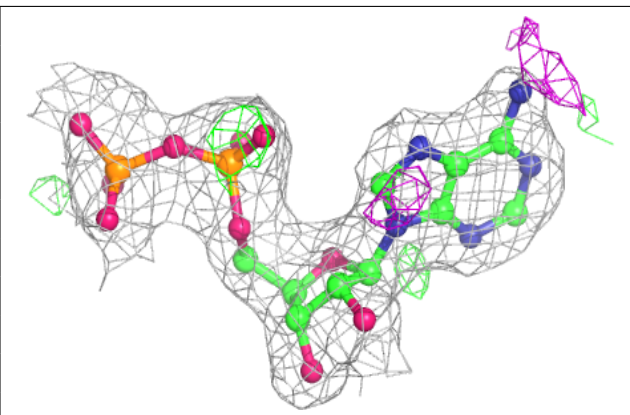mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAD D 601 (A):

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

Electron density around 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)
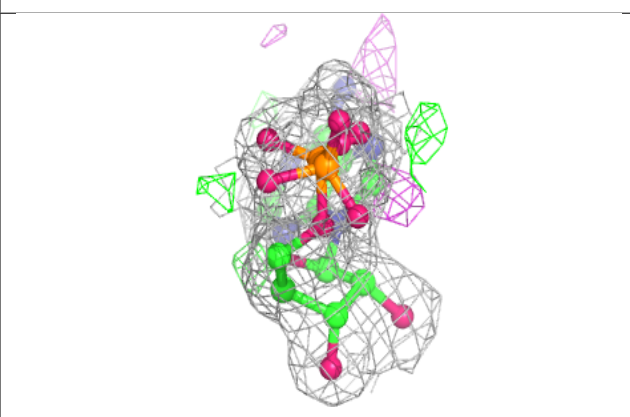
6.5 Other polymers (i)

There are no such residues in this entry.