



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 PM UTC

PDB ID : 8J3O / pdb_00008j3o
Title : Formate dehydrogenase wild-type enzyme from *Candida dubliniensis* complexed with NADH
Authors : Ma, W.; Zheng, Y.C.; Geng, Q.; Chen, C.
Deposited on : 2023-04-17
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

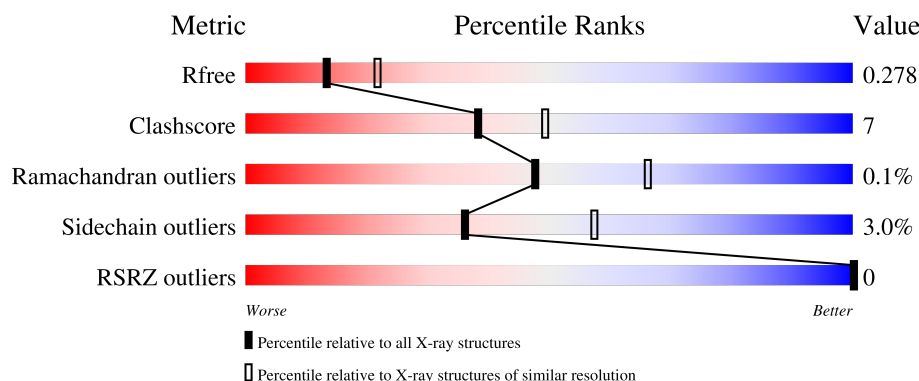
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	 78% 17% . .
1	B	386	 83% 12% . .
1	C	386	 80% 13% . 5%
1	D	386	 75% 18% . 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11731 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2900	1847	490	551	12			
1	B	373	Total	C	N	O	S	0	1	0
			2915	1855	495	553	12			
1	C	367	Total	C	N	O	S	0	0	0
			2858	1820	484	542	12			
1	D	365	Total	C	N	O	S	0	0	0
			2841	1808	482	539	12			

There are 28 discrepancies between the modelled and reference sequences:

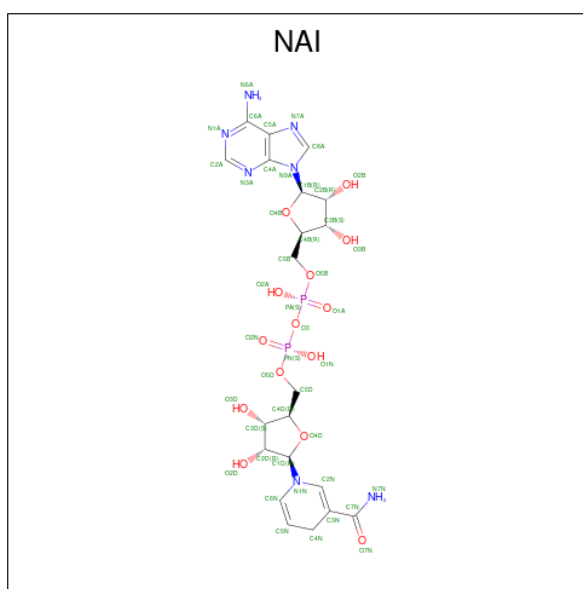
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP B9WHT3
A	-5	HIS	-	expression tag	UNP B9WHT3
A	-4	HIS	-	expression tag	UNP B9WHT3
A	-3	HIS	-	expression tag	UNP B9WHT3
A	-2	HIS	-	expression tag	UNP B9WHT3
A	-1	HIS	-	expression tag	UNP B9WHT3
A	0	HIS	-	expression tag	UNP B9WHT3
B	-6	MET	-	initiating methionine	UNP B9WHT3
B	-5	HIS	-	expression tag	UNP B9WHT3
B	-4	HIS	-	expression tag	UNP B9WHT3
B	-3	HIS	-	expression tag	UNP B9WHT3
B	-2	HIS	-	expression tag	UNP B9WHT3
B	-1	HIS	-	expression tag	UNP B9WHT3
B	0	HIS	-	expression tag	UNP B9WHT3
C	-6	MET	-	initiating methionine	UNP B9WHT3
C	-5	HIS	-	expression tag	UNP B9WHT3
C	-4	HIS	-	expression tag	UNP B9WHT3
C	-3	HIS	-	expression tag	UNP B9WHT3
C	-2	HIS	-	expression tag	UNP B9WHT3
C	-1	HIS	-	expression tag	UNP B9WHT3
C	0	HIS	-	expression tag	UNP B9WHT3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP B9WHT3
D	-5	HIS	-	expression tag	UNP B9WHT3
D	-4	HIS	-	expression tag	UNP B9WHT3
D	-3	HIS	-	expression tag	UNP B9WHT3
D	-2	HIS	-	expression tag	UNP B9WHT3
D	-1	HIS	-	expression tag	UNP B9WHT3
D	0	HIS	-	expression tag	UNP B9WHT3

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (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
			26	10	1	13	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

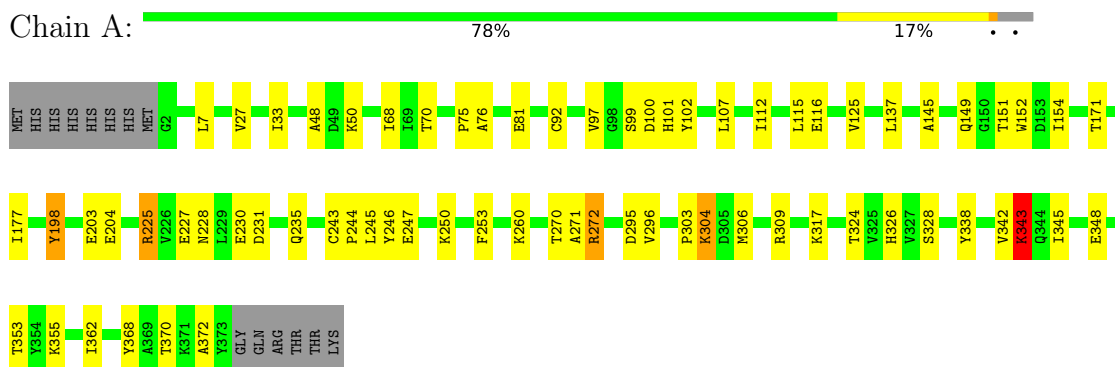
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	16	Total 16	O 16	0	0
4	C	7	Total 7	O 7	0	0
4	D	18	Total 18	O 18	0	0

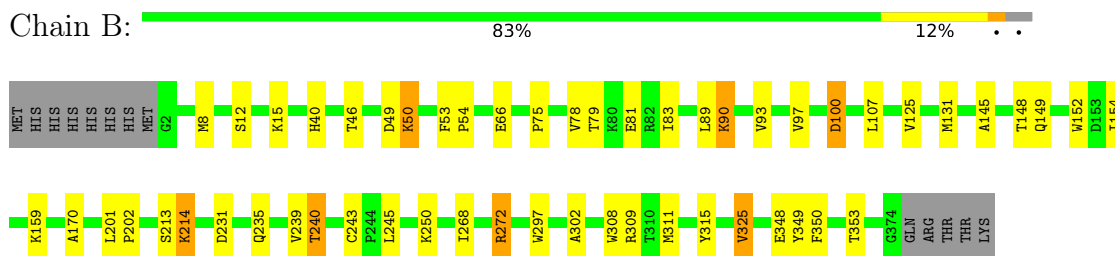
3 Residue-property plots

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.

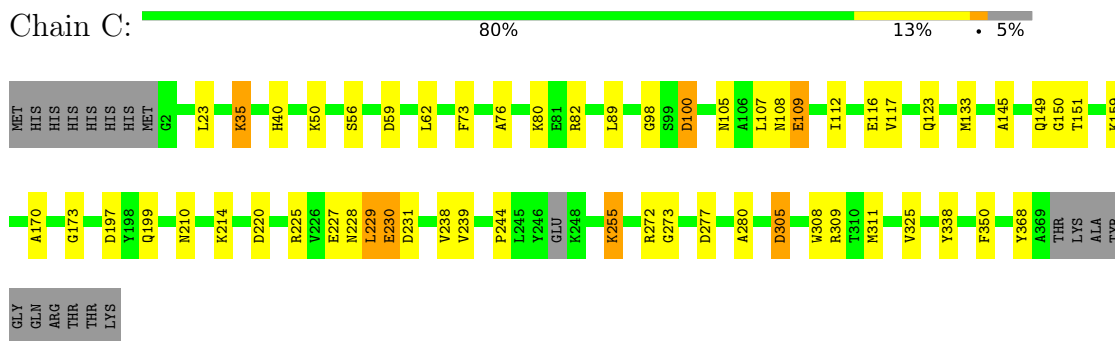
- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase



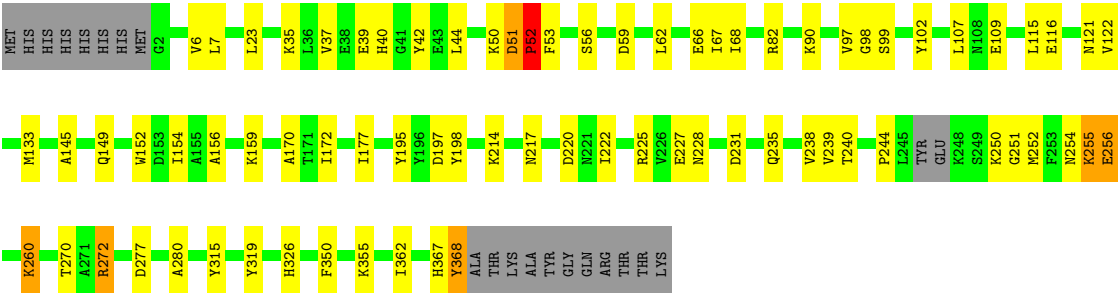
- Molecule 1: Formate dehydrogenase

Chain D:

75%

18%

• 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.40Å 60.16Å 120.48Å 90.00° 90.00° 111.02°	Depositor
Resolution (Å)	44.58 – 2.65 44.58 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (44.58-2.65) 98.1 (44.58-2.65)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.226 , 0.278 0.226 , 0.278	Depositor DCC
R_{free} test set	1792 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.408 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11731	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/2963	0.62	12/4019 (0.3%)
1	B	0.29	0/2978	0.76	12/4038 (0.3%)
1	C	0.25	0/2919	0.67	14/3958 (0.4%)
1	D	0.34	1/2901 (0.0%)	0.74	13/3933 (0.3%)
All	All	0.28	1/11761 (0.0%)	0.70	51/15948 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	260	LYS	CE-NZ	5.96	1.67	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	LEU	CA-C-N	16.60	147.73	122.17
1	B	89	LEU	C-N-CA	16.60	147.73	122.17
1	D	52	PRO	CA-N-CD	-14.36	91.89	112.00
1	D	52	PRO	CB-CA-C	10.97	129.65	111.56
1	D	260	LYS	CD-CE-NZ	-10.91	77.00	111.90
1	C	255	LYS	CG-CD-CE	-10.82	86.40	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	LYS	CB-CA-C	-10.46	94.07	110.81
1	A	204	GLU	CB-CA-C	8.64	123.59	109.07
1	D	260	LYS	CG-CD-CE	8.41	130.65	111.30
1	B	15	LYS	CA-CB-CG	8.36	130.82	114.10
1	B	90	LYS	CA-CB-CG	8.11	130.33	114.10
1	B	15	LYS	CB-CG-CD	-8.06	92.77	111.30
1	C	229	LEU	CA-C-N	7.88	131.62	120.28
1	C	229	LEU	C-N-CA	7.88	131.62	120.28
1	B	15	LYS	CG-CD-CE	-7.82	93.31	111.30
1	A	355	LYS	CA-CB-CG	-7.75	98.60	114.10
1	C	35	LYS	CA-CB-CG	7.68	129.47	114.10
1	C	230	GLU	CB-CG-CD	7.56	125.46	112.60
1	D	260	LYS	CB-CG-CD	7.43	128.38	111.30
1	A	343	LYS	CG-CD-CE	7.21	127.88	111.30
1	D	90	LYS	CB-CG-CD	7.00	127.39	111.30
1	A	204	GLU	N-CA-C	-6.85	105.20	113.97
1	B	15	LYS	CD-CE-NZ	-6.79	90.16	111.90
1	B	90	LYS	CD-CE-NZ	-6.78	90.21	111.90
1	A	304	LYS	CA-CB-CG	6.73	127.57	114.10
1	D	53	PHE	CA-C-O	-6.70	113.20	120.17
1	B	325	VAL	CG1-CB-CG2	6.69	125.52	110.80
1	C	255	LYS	CB-CG-CD	6.64	126.58	111.30
1	A	204	GLU	N-CA-CB	-6.64	101.44	110.67
1	C	35	LYS	CG-CD-CE	-6.61	96.09	111.30
1	C	109	GLU	CB-CA-C	-6.42	98.75	110.63
1	A	343	LYS	CB-CG-CD	6.24	125.65	111.30
1	C	255	LYS	N-CA-CB	6.21	119.19	109.94
1	D	260	LYS	N-CA-CB	-6.12	101.07	110.44
1	D	260	LYS	CA-CB-CG	-6.00	102.10	114.10
1	C	109	GLU	N-CA-CB	5.87	119.27	110.22
1	B	214	LYS	CG-CD-CE	5.79	124.62	111.30
1	B	325	VAL	CA-CB-CG2	5.78	120.22	110.40
1	D	51	ASP	CA-C-N	5.57	126.80	119.84
1	D	51	ASP	C-N-CA	5.57	126.80	119.84
1	C	230	GLU	N-CA-CB	-5.55	101.67	110.22
1	C	35	LYS	N-CA-CB	-5.50	102.03	110.12
1	D	90	LYS	CA-CB-CG	-5.50	103.10	114.10
1	A	198	TYR	CB-CA-C	-5.44	99.07	110.17
1	B	90	LYS	CG-CD-CE	5.36	123.64	111.30
1	D	270	THR	N-CA-C	-5.30	106.12	112.59
1	A	204	GLU	CA-CB-CG	5.29	124.68	114.10
1	C	230	GLU	N-CA-C	5.28	117.78	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	TYR	CA-CB-CG	5.10	123.07	113.90
1	A	355	LYS	CD-CE-NZ	-5.07	95.67	111.90
1	A	304	LYS	CG-CD-CE	-5.02	99.75	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	GLU	Peptide
1	A	225	ARG	Sidechain
1	C	109	GLU	Sidechain

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	2900	0	2888	47	0
1	B	2915	0	2903	35	1
1	C	2858	0	2847	36	1
1	D	2841	0	2832	45	0
2	A	44	0	27	5	0
2	B	44	0	27	6	0
2	C	26	0	15	3	0
2	D	44	0	26	7	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	0	0	1
4	B	16	0	0	0	0
4	C	7	0	0	0	0
4	D	18	0	0	2	1
All	All	11731	0	11565	161	2

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 7.

All (161) 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:D:109:GLU:OE2	4:D:501:HOH:O	1.91	0.86
1:A:225:ARG:NH1	1:A:227:GLU:HG2	1.94	0.83
1:B:50:LYS:NZ	1:B:75:PRO:O	2.13	0.82
1:A:244:PRO:HD3	2:A:401:NAI:H51A	1.61	0.80
1:C:62:LEU:HD11	1:C:82:ARG:HG2	1.68	0.76
1:C:100:ASP:OD2	1:C:272:ARG:HD3	1.87	0.74
1:A:198:TYR:OH	1:A:246:TYR:CZ	2.40	0.73
1:D:159:LYS:HD2	1:D:315:TYR:CZ	2.27	0.70
1:A:151:THR:O	1:C:309:ARG:NH2	2.25	0.69
1:D:62:LEU:HD11	1:D:82:ARG:HG2	1.74	0.68
1:A:198:TYR:OH	1:A:246:TYR:OH	1.82	0.67
1:A:225:ARG:HH12	1:A:227:GLU:HG2	1.58	0.67
1:C:228:ASN:OD1	1:C:230:GLU:HG2	1.95	0.66
1:D:197:ASP:OD1	2:D:401:NAI:O2B	2.12	0.66
1:D:256:GLU:O	1:D:260:LYS:HG3	1.95	0.66
1:B:79:THR:O	1:B:83:ILE:HG12	1.96	0.66
1:D:177:ILE:HD12	2:D:401:NAI:H51N	1.76	0.66
1:B:201:LEU:HD23	1:B:202:PRO:HD2	1.77	0.65
1:A:107:LEU:HD22	1:A:112:ILE:HG21	1.80	0.64
1:B:125:VAL:HG11	2:B:401:NAI:H5N	1.80	0.63
1:C:214:LYS:HG2	1:C:220:ASP:HA	1.78	0.63
1:A:33:ILE:HG22	1:A:343:LYS:HG3	1.79	0.63
1:C:305:ASP:N	1:C:305:ASP:OD1	2.32	0.62
1:A:145:ALA:O	1:A:149:GLN:HG2	1.98	0.62
1:A:245:LEU:HD11	1:A:250:LYS:HD2	1.82	0.62
1:B:125:VAL:HG21	2:B:401:NAI:H42N	1.82	0.61
1:B:152:TRP:NE1	1:B:154:ILE:HD11	2.16	0.60
1:C:105:ASN:HA	1:C:108:ASN:HB2	1.84	0.58
1:A:115:LEU:HB3	1:A:345:ILE:HD13	1.85	0.58
1:B:245:LEU:HD11	1:B:250:LYS:HD2	1.86	0.58
1:A:152:TRP:NE1	1:A:154:ILE:HD11	2.19	0.57
1:C:228:ASN:OD1	1:C:231:ASP:N	2.37	0.57
1:A:309:ARG:NH2	1:C:151:THR:O	2.36	0.57
1:C:225:ARG:HH11	1:C:227:GLU:HG2	1.68	0.57
1:C:197:ASP:HB3	1:C:199:GLN:O	2.05	0.56
1:D:172:ILE:HG21	1:D:252:MET:HE1	1.88	0.56
1:D:98:GLY:N	1:D:116:GLU:OE2	2.36	0.56
1:C:225:ARG:NH1	1:C:227:GLU:HG2	2.21	0.56
1:D:116:GLU:CD	1:D:362:ILE:HD11	2.30	0.56
1:A:50:LYS:NZ	1:A:75:PRO:O	2.27	0.55
1:A:230:GLU:CG	1:A:260:LYS:HD3	2.36	0.54
1:B:308:TRP:HA	1:B:311:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:HG12	1:B:83:ILE:HD11	1.90	0.53
1:D:145:ALA:O	1:D:149:GLN:HG2	2.09	0.53
1:D:326:HIS:HE2	2:D:401:NAI:C7N	2.22	0.53
1:D:97:VAL:HB	2:D:401:NAI:H5N	1.90	0.53
1:D:367:HIS:O	1:D:368:TYR:HD1	1.92	0.53
1:B:83:ILE:HD12	1:B:107:LEU:HD21	1.92	0.52
1:A:244:PRO:HD2	2:A:401:NAI:C8A	2.39	0.52
1:D:170:ALA:O	1:D:239:VAL:HA	2.10	0.52
1:D:152:TRP:NE1	1:D:154:ILE:HD11	2.25	0.52
1:C:145:ALA:O	1:C:149:GLN:HG2	2.10	0.51
1:A:198:TYR:CZ	1:A:246:TYR:OH	2.54	0.51
1:D:51:ASP:HB3	1:D:52:PRO:HD2	1.92	0.50
1:C:308:TRP:HA	1:C:311:MET:HE2	1.93	0.50
1:D:217:ASN:ND2	4:D:502:HOH:O	2.27	0.50
1:D:122:VAL:HG12	1:D:177:ILE:HG13	1.93	0.50
1:B:83:ILE:HD12	1:B:107:LEU:CD2	2.42	0.50
1:D:198:TYR:CZ	2:D:401:NAI:C5A	2.94	0.50
1:B:170:ALA:O	1:B:239:VAL:HA	2.12	0.50
1:D:37:VAL:HG11	1:D:44:LEU:HB2	1.93	0.49
1:A:27:VAL:HG21	1:A:48:ALA:HB2	1.94	0.49
1:B:81:GLU:H	1:B:81:GLU:CD	2.21	0.49
1:D:56:SER:OG	1:D:59:ASP:OD2	2.27	0.49
1:B:302:ALA:O	1:B:309:ARG:NH1	2.46	0.49
1:B:83:ILE:CD1	1:B:107:LEU:HD21	2.43	0.48
1:D:99:SER:HB3	1:D:102:TYR:HD2	1.78	0.48
1:D:42:TYR:OH	1:D:66:GLU:OE2	2.18	0.48
1:C:277:ASP:HB3	1:C:280:ALA:HB3	1.95	0.48
1:A:370:THR:HG23	1:A:372:ALA:H	1.79	0.48
1:B:159:LYS:HD2	1:B:315:TYR:CZ	2.49	0.48
1:A:230:GLU:HG2	1:A:260:LYS:HD3	1.96	0.48
1:D:255:LYS:HB3	1:D:255:LYS:HE3	1.48	0.48
1:A:198:TYR:CE1	1:A:246:TYR:OH	2.67	0.47
1:C:40:HIS:CD2	1:C:350:PHE:HB3	2.49	0.47
1:C:210:ASN:O	1:C:214:LYS:HG3	2.14	0.47
1:D:250:LYS:HD3	1:D:251:GLY:N	2.29	0.47
1:C:228:ASN:HB3	1:C:231:ASP:HB2	1.97	0.47
1:D:40:HIS:CD2	1:D:350:PHE:HB3	2.50	0.47
1:D:156:ALA:O	1:D:319:TYR:OH	2.28	0.47
1:B:348:GLU:OE1	1:B:353:THR:OG1	2.33	0.47
1:C:229:LEU:HB3	1:C:230:GLU:OE2	2.14	0.46
1:B:66:GLU:CG	1:B:90:LYS:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:OG	1:C:59:ASP:OD2	2.32	0.46
1:D:159:LYS:HD2	1:D:315:TYR:CE1	2.50	0.46
1:A:272:ARG:HD3	1:A:272:ARG:HA	1.59	0.46
1:C:228:ASN:OD1	1:C:230:GLU:CG	2.64	0.46
1:B:231:ASP:O	1:B:235:GLN:HG3	2.16	0.46
1:C:117:VAL:HG11	1:C:338:TYR:HA	1.96	0.46
1:A:243:CYS:HB2	2:A:401:NAI:C5A	2.45	0.46
1:D:159:LYS:HD2	1:D:315:TYR:CE2	2.50	0.46
1:A:348:GLU:OE1	1:A:353:THR:OG1	2.33	0.46
1:A:230:GLU:HG3	1:A:260:LYS:HD3	1.97	0.46
1:A:97:VAL:HB	2:A:401:NAI:H5N	1.97	0.46
1:B:90:LYS:HD2	1:B:349:TYR:OH	2.16	0.46
1:A:304:LYS:HG2	1:C:150:GLY:O	2.15	0.45
1:A:70:THR:OG1	1:A:101:HIS:NE2	2.42	0.45
1:D:98:GLY:HA3	1:D:272:ARG:HH12	1.82	0.45
1:B:159:LYS:HE2	1:B:159:LYS:HB3	1.65	0.45
1:A:125:VAL:HB	1:A:177:ILE:HD13	1.98	0.45
1:B:53:PHE:CE1	1:B:54:PRO:HB3	2.51	0.45
1:A:50:LYS:HD2	1:A:76:ALA:HA	1.99	0.45
1:C:173:GLY:HA2	2:C:401:NAI:H1B	1.98	0.45
1:A:231:ASP:O	1:A:235:GLN:HG3	2.17	0.45
1:B:8:MET:HG2	1:B:46:THR:HG23	1.98	0.45
1:B:81:GLU:CD	1:B:81:GLU:N	2.75	0.45
1:D:231:ASP:C	1:D:235:GLN:HE21	2.25	0.45
1:D:277:ASP:HB3	1:D:280:ALA:HB3	1.98	0.45
1:A:326:HIS:HE2	2:A:401:NAI:C7N	2.30	0.44
1:A:100:ASP:HB2	1:A:245:LEU:HD23	2.00	0.44
1:A:338:TYR:O	1:A:342:VAL:HG23	2.18	0.44
1:B:100:ASP:OD1	1:B:272[B]:ARG:HD3	2.18	0.44
1:D:133:MET:HG2	1:D:238:VAL:HG11	1.98	0.44
1:A:81:GLU:H	1:A:81:GLU:CD	2.26	0.44
1:C:197:ASP:CG	2:C:401:NAI:HO2A	2.25	0.44
2:B:401:NAI:H51N	2:B:401:NAI:H6N	2.00	0.43
1:C:133:MET:HG2	1:C:238:VAL:HG11	1.98	0.43
1:C:244:PRO:HD3	2:C:401:NAI:H52A	2.00	0.43
1:D:35:LYS:HD3	1:D:39:GLU:OE1	2.18	0.43
1:C:123:GLN:H	1:C:123:GLN:CD	2.27	0.43
1:A:303:PRO:O	1:A:306:MET:HB2	2.17	0.43
1:B:131:MET:HE2	1:B:131:MET:HB3	1.79	0.43
1:D:195:TYR:CZ	1:D:225:ARG:HB2	2.54	0.43
1:B:40:HIS:ND1	1:B:350:PHE:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:THR:HA	1:B:268:ILE:O	2.19	0.43
1:D:244:PRO:HD2	2:D:401:NAI:N3A	2.34	0.43
1:A:271:ALA:O	1:A:296:VAL:HG11	2.19	0.43
1:D:121:ASN:HD21	2:D:401:NAI:H5N	1.84	0.43
1:B:152:TRP:CD1	1:B:154:ILE:HD11	2.54	0.42
1:B:272[A]:ARG:NH1	1:B:297:TRP:O	2.52	0.42
1:D:102:TYR:HB3	1:D:107:LEU:HD11	2.01	0.42
1:C:98:GLY:N	1:C:116:GLU:OE2	2.43	0.42
1:C:170:ALA:O	1:C:239:VAL:HA	2.20	0.42
1:D:367:HIS:O	1:D:368:TYR:CD1	2.70	0.42
1:B:66:GLU:HG2	1:B:90:LYS:HG3	2.02	0.42
1:B:97:VAL:O	2:B:401:NAI:N7N	2.52	0.42
1:A:99:SER:HB3	1:A:102:TYR:HD2	1.85	0.42
1:A:228:ASN:OD1	1:A:231:ASP:OD1	2.38	0.42
1:B:145:ALA:O	1:B:149:GLN:HG2	2.20	0.42
1:C:107:LEU:HB3	1:C:112:ILE:HB	2.02	0.42
1:D:6:VAL:HG22	1:D:67:ILE:HB	2.01	0.42
1:A:92:CYS:HB3	1:A:102:TYR:CE1	2.54	0.41
1:C:272:ARG:HA	1:C:272:ARG:HD2	1.78	0.41
1:C:272:ARG:NH1	1:C:273:GLY:H	2.18	0.41
1:D:23:LEU:HD12	1:D:23:LEU:HA	1.89	0.41
1:A:295:ASP:OD2	1:A:328:SER:HB3	2.20	0.41
1:B:125:VAL:CG2	2:B:401:NAI:H42N	2.48	0.41
1:C:89:LEU:HD12	1:C:112:ILE:HG21	2.02	0.41
1:D:7:LEU:O	1:D:68:ILE:HA	2.20	0.41
1:D:214:LYS:HG2	1:D:220:ASP:HA	2.02	0.41
1:D:228:ASN:HB3	1:D:231:ASP:CG	2.46	0.41
1:A:125:VAL:HG22	1:A:328:SER:OG	2.20	0.41
1:A:225:ARG:HH11	1:A:227:GLU:HG2	1.79	0.41
1:A:295:ASP:HA	1:A:324:THR:O	2.20	0.41
1:B:243:CYS:HB2	2:B:401:NAI:C5A	2.51	0.41
1:A:317:LYS:HB3	1:A:317:LYS:HE3	1.67	0.41
1:A:7:LEU:O	1:A:68:ILE:HA	2.21	0.40
1:C:50:LYS:HD2	1:C:76:ALA:HA	2.03	0.40
1:C:159:LYS:HE3	1:C:159:LYS:HB3	1.83	0.40
1:D:225:ARG:HE	1:D:227:GLU:HG2	1.86	0.40
1:A:116:GLU:OE1	1:A:362:ILE:HD11	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASP:OD2	1:C:80:LYS:NZ[1_545]	1.95	0.25
4:A:511:HOH:O	4:D:501:HOH:O[1_556]	2.10	0.10

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	370/386 (96%)	356 (96%)	14 (4%)	0	100	100
1	B	372/386 (96%)	358 (96%)	14 (4%)	0	100	100
1	C	363/386 (94%)	349 (96%)	14 (4%)	0	100	100
1	D	361/386 (94%)	345 (96%)	14 (4%)	2 (1%)	21	34
All	All	1466/1544 (95%)	1408 (96%)	56 (4%)	2 (0%)	48	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	52	PRO
1	D	256	GLU

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	307/320 (96%)	299 (97%)	8 (3%)	40	63
1	B	308/320 (96%)	297 (96%)	11 (4%)	31	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	303/320 (95%)	295 (97%)	8 (3%)	40	63
1	D	302/320 (94%)	292 (97%)	10 (3%)	33	55
All	All	1220/1280 (95%)	1183 (97%)	37 (3%)	36	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	171	THR
1	A	247	GLU
1	A	253	PHE
1	A	270	THR
1	A	272	ARG
1	A	343	LYS
1	A	368	TYR
1	B	12	SER
1	B	50	LYS
1	B	93	VAL
1	B	100	ASP
1	B	148	THR
1	B	213	SER
1	B	214	LYS
1	B	240	THR
1	B	272[A]	ARG
1	B	272[B]	ARG
1	B	325	VAL
1	C	23	LEU
1	C	35	LYS
1	C	73	PHE
1	C	100	ASP
1	C	255	LYS
1	C	305	ASP
1	C	325	VAL
1	C	368	TYR
1	D	50	LYS
1	D	52	PRO
1	D	115	LEU
1	D	222	ILE
1	D	240	THR
1	D	254	ASN
1	D	255	LYS

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Mol	Chain	Res	Type
1	D	272	ARG
1	D	355	LYS
1	D	368	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	235	GLN
1	A	242	ASN
1	A	300	GLN
1	A	313	ASN
1	A	367	HIS
1	B	144	HIS
1	B	235	GLN
1	B	313	ASN
1	B	367	HIS
1	C	217	ASN
1	C	242	ASN
1	C	279	GLN
1	C	313	ASN
1	D	217	ASN
1	D	242	ASN
1	D	289	HIS
1	D	313	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	NAI	A	401	-	47,48,48	0.25	0	64,73,73	0.40	0
2	NAI	B	401	-	47,48,48	0.24	0	64,73,73	0.54	1 (1%)
2	NAI	D	401	-	47,48,48	0.31	0	64,73,73	0.51	0
2	NAI	C	401	-	26,27,48	0.37	0	34,41,73	0.55	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	NAI	A	401	-	-	8/29/72/72	0/5/5/5
2	NAI	B	401	-	-	13/29/72/72	0/5/5/5
2	NAI	D	401	-	-	16/29/72/72	0/5/5/5
2	NAI	C	401	-	-	10/18/47/72	0/2/2/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAI	C3N-C2N-N1N	-3.19	118.52	123.20

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C5D-O5D-PN-O3
2	A	401	NAI	C5D-O5D-PN-O1N
2	B	401	NAI	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	401	NAI	C5B-O5B-PA-O3
2	B	401	NAI	C2N-C3N-C7N-N7N
2	C	401	NAI	C5B-O5B-PA-O1A
2	C	401	NAI	C5B-O5B-PA-O2A
2	C	401	NAI	C5B-O5B-PA-O3
2	D	401	NAI	C5B-O5B-PA-O1A
2	D	401	NAI	C5B-O5B-PA-O2A
2	D	401	NAI	C5B-O5B-PA-O3
2	D	401	NAI	C5D-O5D-PN-O3
2	D	401	NAI	C5D-O5D-PN-O2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	O4D-C4D-C5D-O5D
2	A	401	NAI	C3D-C4D-C5D-O5D
2	D	401	NAI	O4D-C4D-C5D-O5D
2	D	401	NAI	C3D-C4D-C5D-O5D
2	D	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C3B-C4B-C5B-O5B
2	D	401	NAI	C3B-C4B-C5B-O5B
2	C	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	C4B-C5B-O5B-PA
2	B	401	NAI	PN-O3-PA-O5B
2	C	401	NAI	PN-O3-PA-O5B
2	D	401	NAI	PN-O3-PA-O5B
2	A	401	NAI	O4B-C4B-C5B-O5B
2	C	401	NAI	C3D-C4D-C5D-O5D
2	D	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	C2B-C1B-N9A-C8A
2	C	401	NAI	PA-O3-PN-O2N
2	D	401	NAI	PA-O3-PN-O1N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	C5B-O5B-PA-O2A
2	B	401	NAI	C5D-O5D-PN-O1N
2	B	401	NAI	O4D-C4D-C5D-O5D
2	A	401	NAI	O4D-C1D-N1N-C2N
2	C	401	NAI	O4D-C4D-C5D-O5D
2	B	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	O4B-C1B-N9A-C8A
2	A	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	PA-O3-PN-O2N
2	B	401	NAI	C2B-C1B-N9A-C4A

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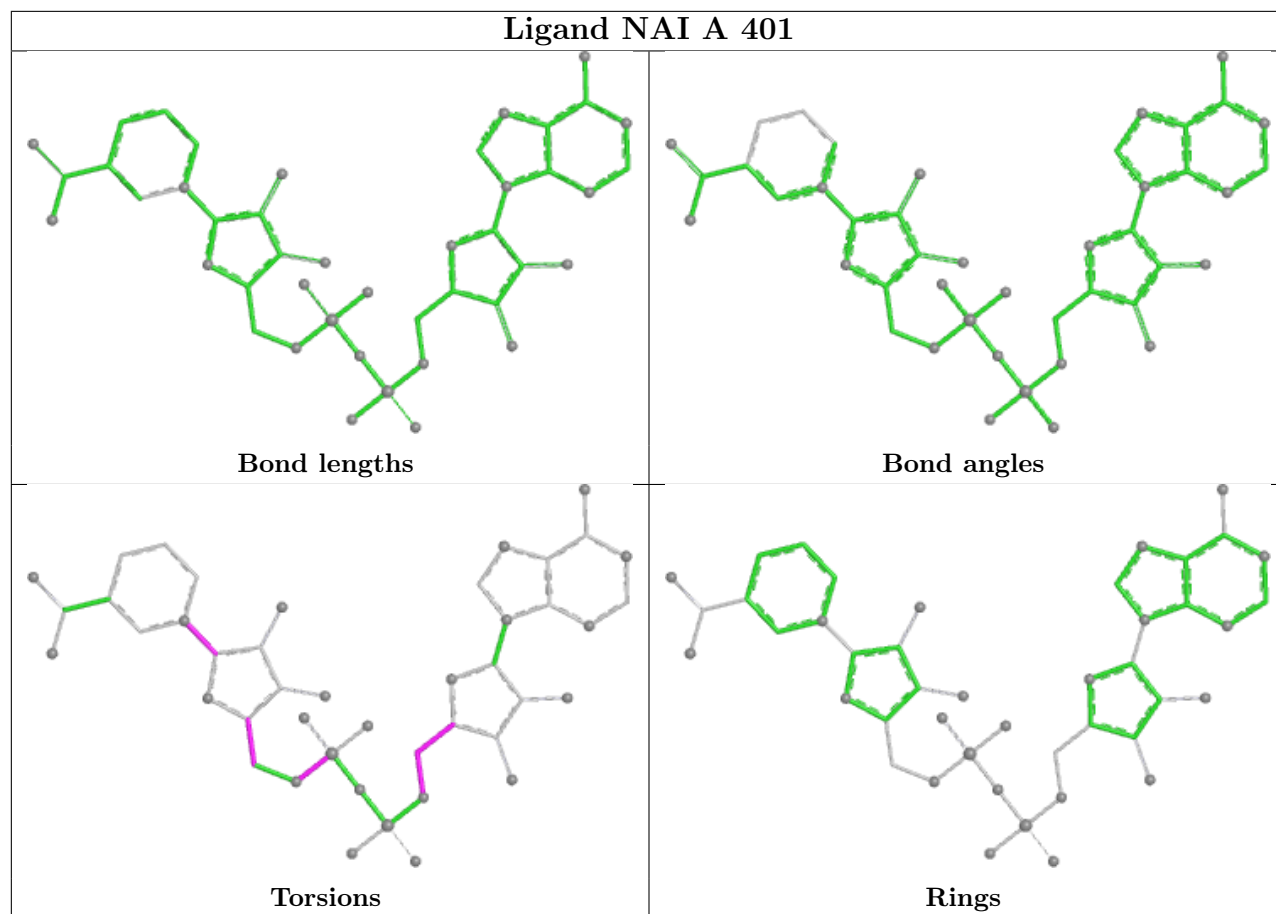
Mol	Chain	Res	Type	Atoms
2	C	401	NAI	PA-O3-PN-O1N
2	B	401	NAI	O4B-C4B-C5B-O5B

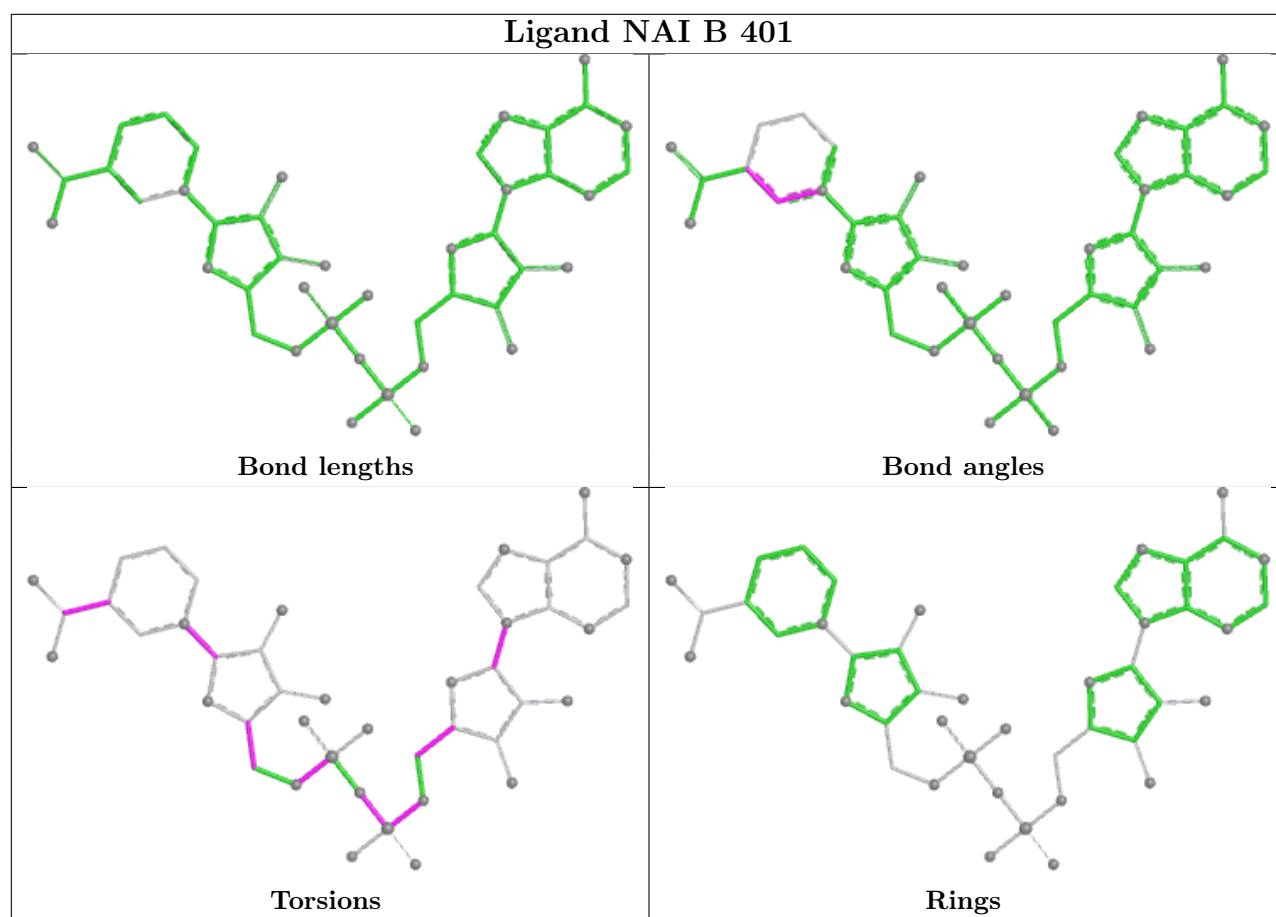
There are no ring outliers.

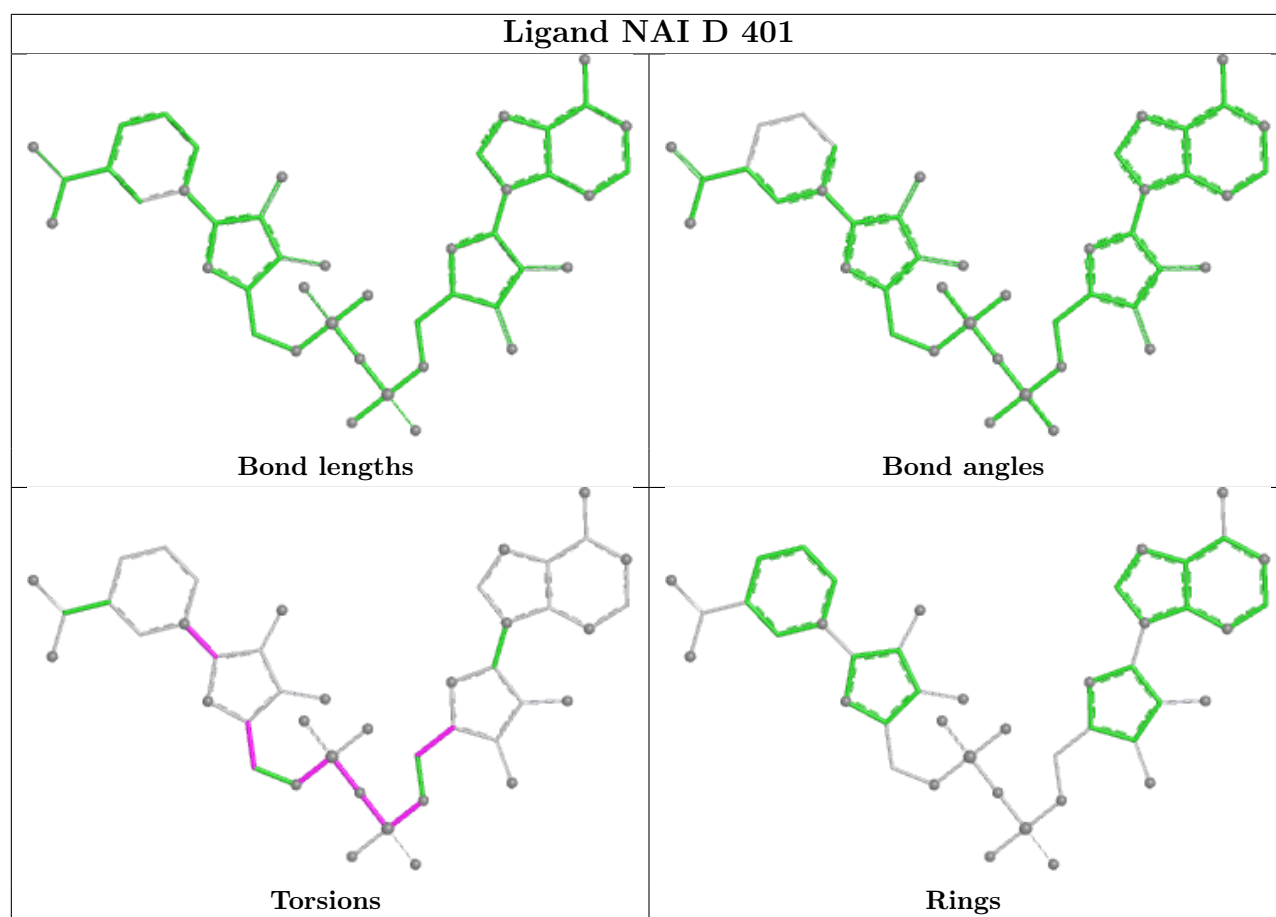
4 monomers are involved in 21 short contacts:

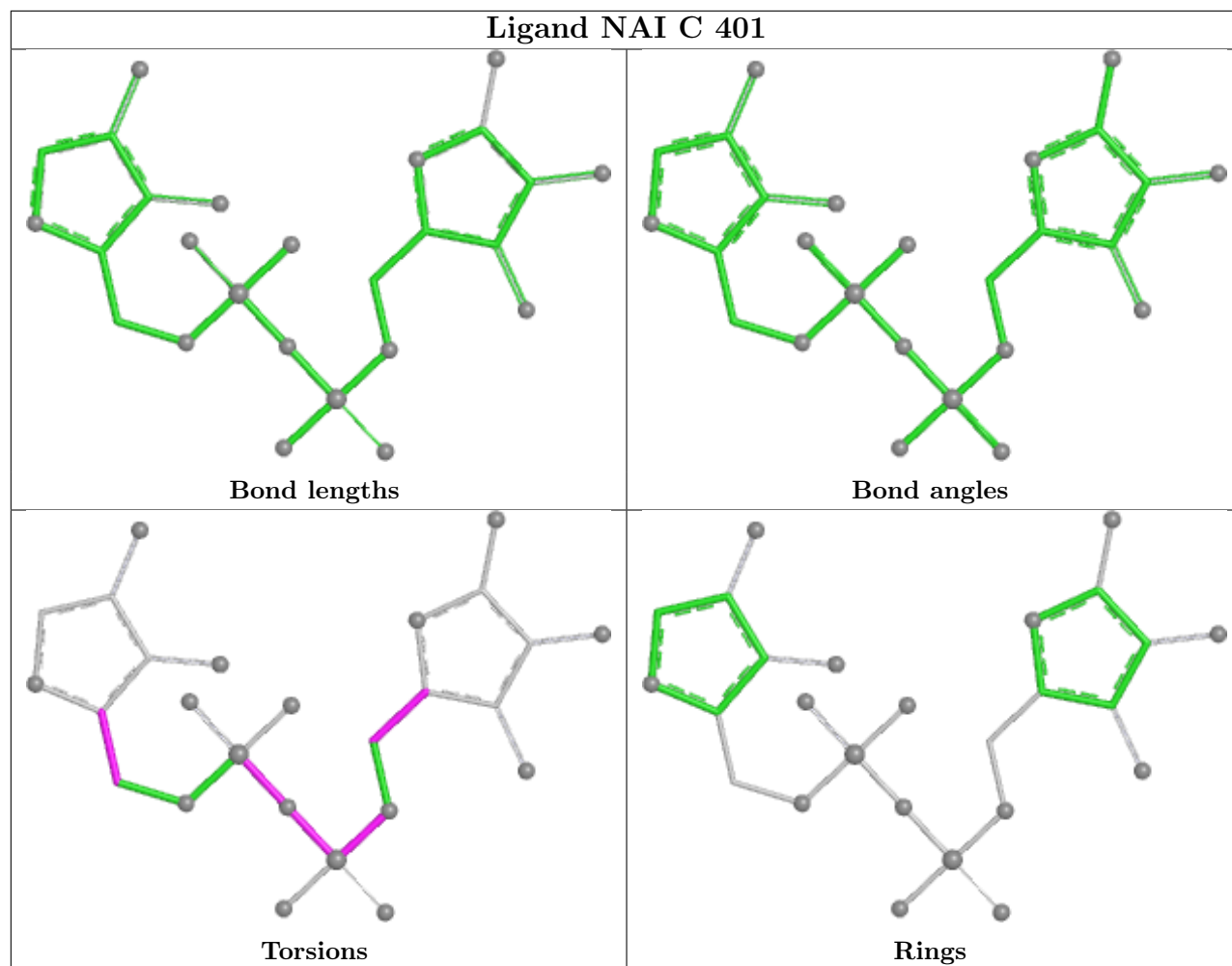
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAI	5	0
2	B	401	NAI	6	0
2	D	401	NAI	7	0
2	C	401	NAI	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 [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	372/386 (96%)	-1.63	0 100 100	33, 45, 70, 108	0
1	B	373/386 (96%)	-1.63	0 100 100	25, 46, 72, 109	1 (0%)
1	C	367/386 (95%)	-1.60	0 100 100	35, 49, 71, 105	0
1	D	365/386 (94%)	-1.63	0 100 100	30, 48, 71, 103	0
All	All	1477/1544 (95%)	-1.62	0 100 100	25, 47, 72, 109	1 (0%)

There are no RSRZ outliers to report.

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
2	NAI	C	401	26/44	0.98	0.04	61,70,75,80	0
2	NAI	D	401	44/44	0.98	0.04	47,70,80,83	0
2	NAI	A	401	44/44	0.99	0.04	41,72,83,101	0
2	NAI	B	401	44/44	0.99	0.04	49,68,76,79	0

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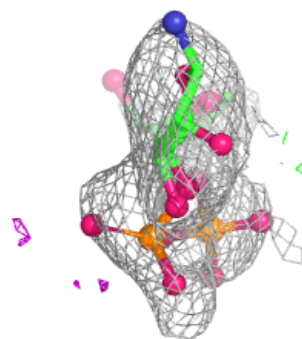
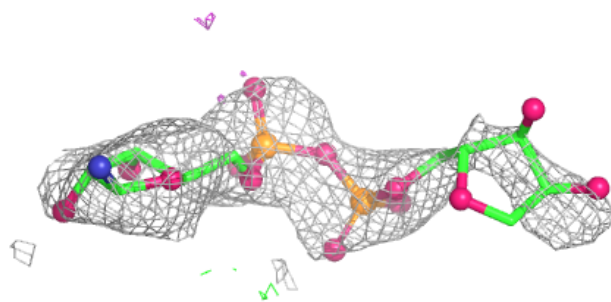
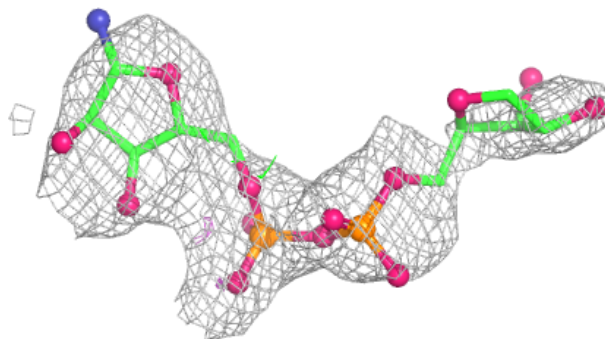
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	402	1/1	0.99	0.02	38,38,38,38	0
3	MG	C	402	1/1	0.99	0.02	39,39,39,39	0
3	MG	D	402	1/1	0.99	0.04	38,38,38,38	0

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.

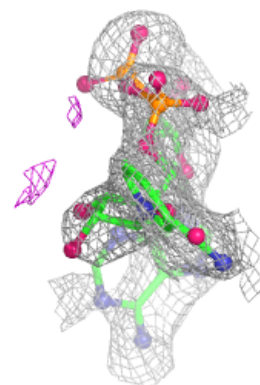
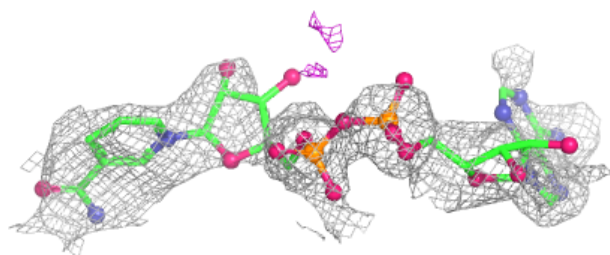
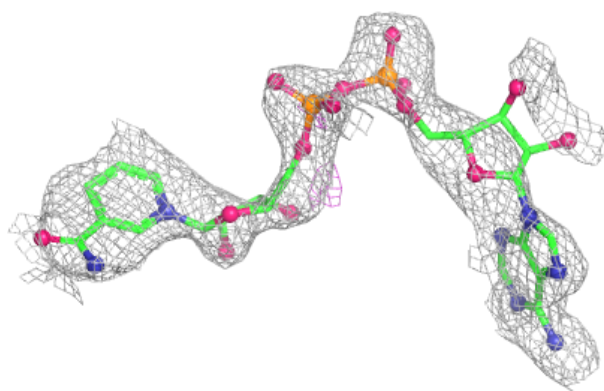
Electron density around NAI C 401:

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

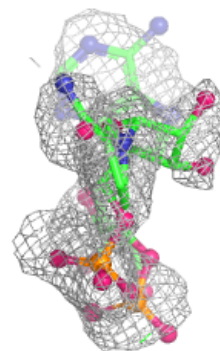
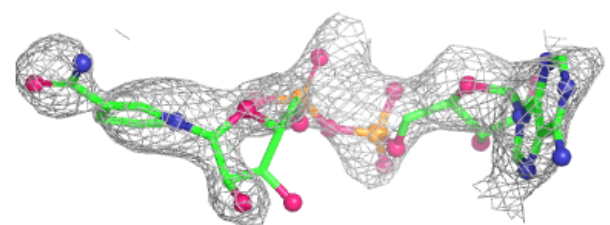
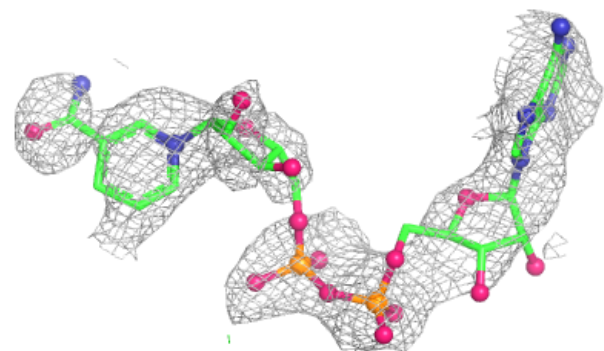


Electron density around NAI D 401:

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

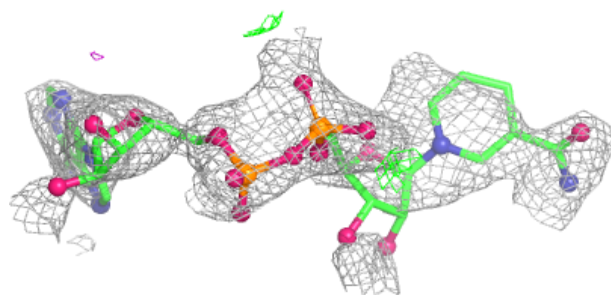
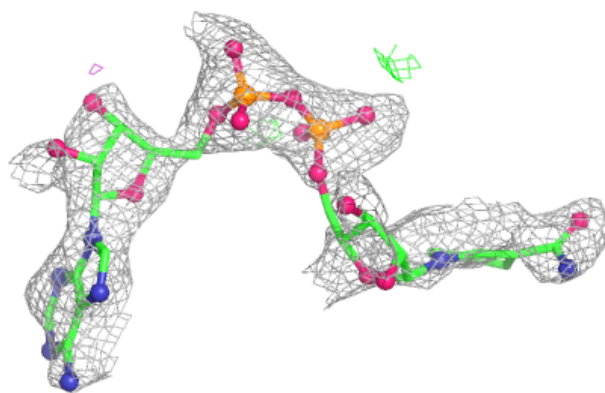
**Electron density around NAI A 401:**

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



Electron density around NAI B 401:

$2mF_o - DF_c$ (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.