



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 PM UTC

PDB ID : 5NQQ / pdb_00005nqq
Title : Rabbit Muscle L-lactate dehydrogenase in complex with NADH and oxaloacetate
Authors : Luisi, B.F.; Olin-Sandoval, V.
Deposited on : 2017-04-20
Resolution : 1.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

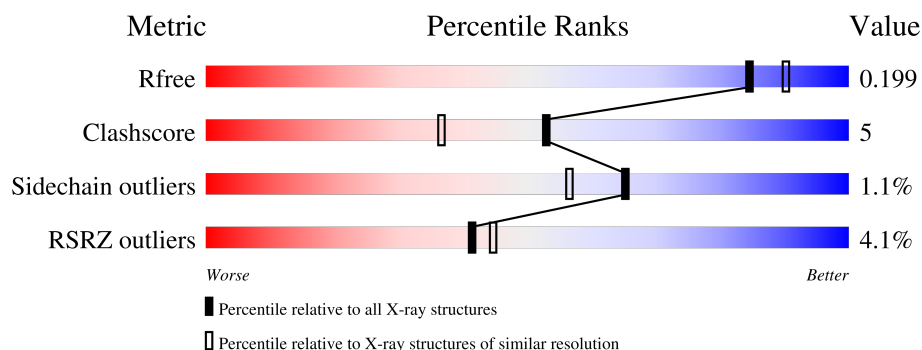
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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

Mol	Chain	Length	Quality of chain
1	A	332	 6% 91% 8%
1	B	332	 3% 91% 8%
1	C	332	 3% 92% 8%
1	D	332	 5% 92% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21786 atoms, of which 10620 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.

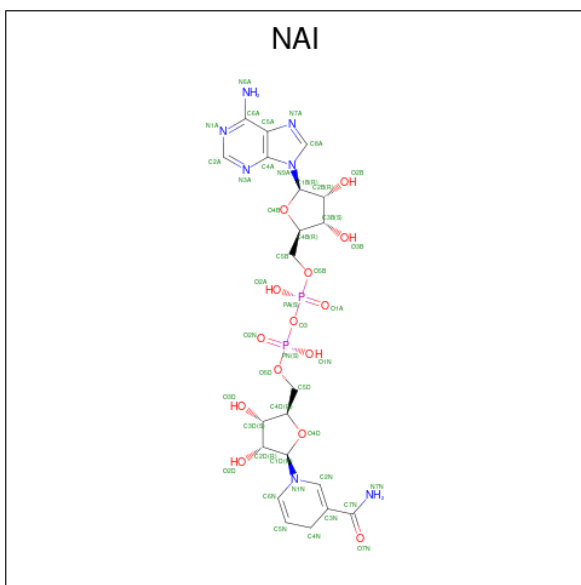
- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	331	Total	C	H	N	O	S	0	1	0
			5154	1625	2611	437	467	14			
1	B	331	Total	C	H	N	O	S	0	2	0
			5179	1630	2629	439	467	14			
1	C	331	Total	C	H	N	O	S	0	2	0
			5223	1639	2654	445	471	14			
1	D	331	Total	C	H	N	O	S	0	3	0
			5153	1627	2614	437	461	14			

There are 4 discrepancies between the modelled and reference sequences:

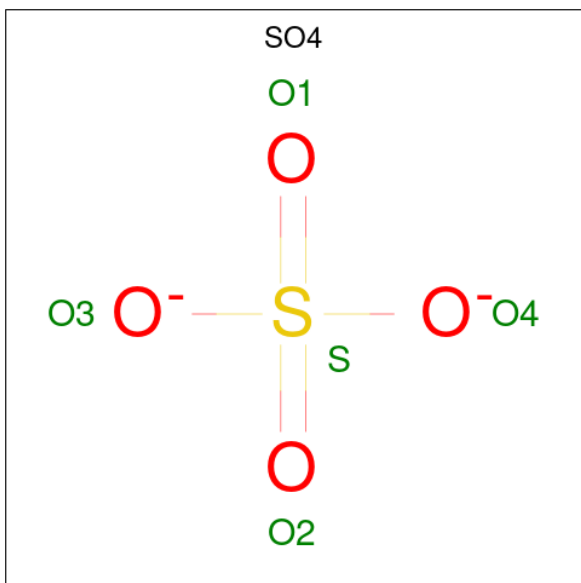
Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	THR	engineered mutation	UNP P13491
B	248	SER	THR	engineered mutation	UNP P13491
C	248	SER	THR	engineered mutation	UNP P13491
D	248	SER	THR	engineered mutation	UNP P13491

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



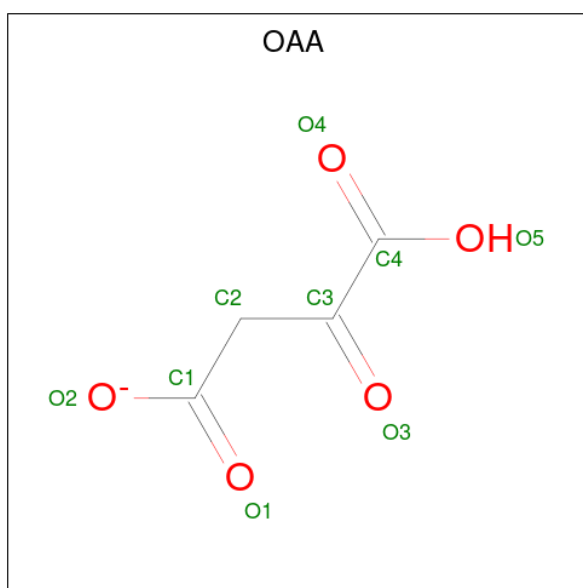
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	B	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	C	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	D	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 11 4 2 5	0	0
4	D	1	Total C H O 11 4 2 5	0	0

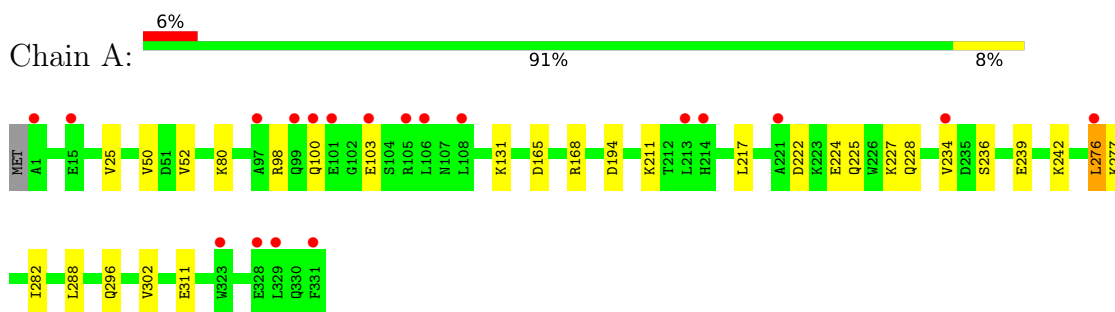
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	179	Total O 179 179	0	0
5	B	184	Total O 184 184	0	0
5	C	203	Total O 203 203	0	0
5	D	185	Total O 185 185	0	0

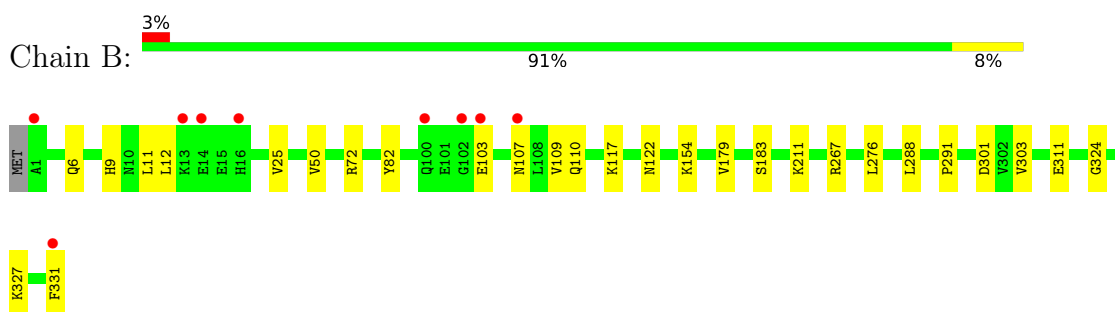
3 Residue-property plots

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.

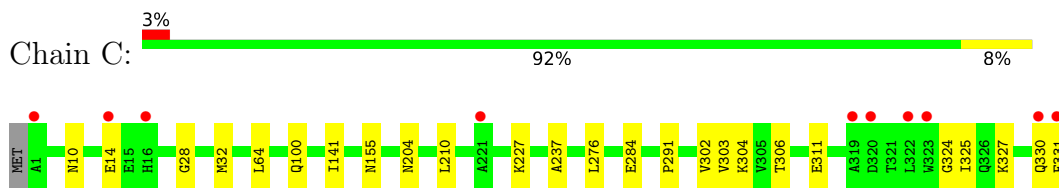
- Molecule 1: L-lactate dehydrogenase A chain



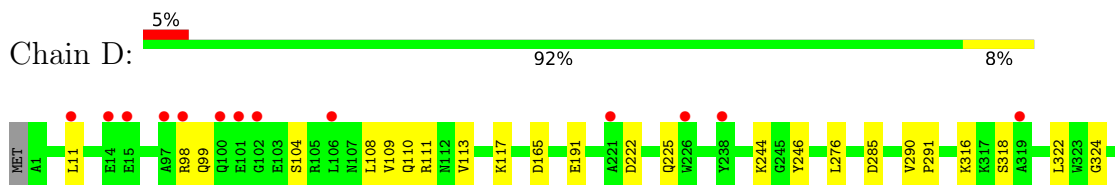
- Molecule 1: L-lactate dehydrogenase A chain

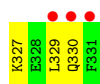


- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain





A vertical color key for residue validation. It consists of a yellow column on the left and a green column on the right. The yellow column contains the labels K327, F328, L329, Q330, and F331. The green column contains the labels F328, L329, Q330, and F331. Above the yellow column, there are three red dots. Above the green column, there are two red dots.

K327	
F328	F328
L329	L329
Q330	Q330
F331	F331

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.37Å 138.76Å 74.57Å 90.00° 110.12° 90.00°	Depositor
Resolution (Å)	29.42 – 1.87 29.42 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.42-1.87) 98.8 (29.42-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.87Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.170 , 0.199 (Not available) , 0.199	Depositor DCC
R_{free} test set	5627 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21786	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: OAA, NAI, SO4

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	0.50	0/2595	0.64	1/3510 (0.0%)
1	B	0.53	0/2603	0.68	0/3521
1	C	0.51	0/2624	0.62	0/3546
1	D	0.53	0/2596	0.67	0/3513
All	All	0.52	0/10418	0.65	1/14090 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	LEU	N-CA-C	6.03	120.63	113.16

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	2543	2611	2615	41	0
1	B	2550	2629	2629	28	0
1	C	2569	2654	2655	21	0
1	D	2539	2614	2616	21	0
2	A	44	27	26	0	0
2	B	44	27	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	27	27	2	0
2	D	44	27	27	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	C	9	2	2	2	0
4	D	9	2	2	0	0
5	A	179	0	0	5	2
5	B	184	0	0	6	2
5	C	203	0	0	7	1
5	D	185	0	0	7	1
All	All	11166	10620	10626	106	3

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 5.

All (106) 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:A:194:ASP:HA	1:A:234:VAL:HG11	1.36	1.07
1:A:100:GLN:CB	1:A:103:GLU:HG3	1.87	1.01
1:D:117:LYS:NZ	5:D:501:HOH:O	1.92	1.01
1:C:100:GLN:NE2	5:C:501:HOH:O	1.96	0.98
1:A:100:GLN:CB	1:A:103:GLU:CG	2.45	0.95
1:A:276:LEU:CD2	1:A:288:LEU:HB2	1.96	0.94
1:A:311:GLU:OE1	5:A:501:HOH:O	1.85	0.94
1:A:276:LEU:HD23	1:A:288:LEU:HB2	1.49	0.92
1:A:276:LEU:HD11	1:A:282:ILE:HG21	1.49	0.92
1:A:276:LEU:HD21	1:A:288:LEU:HD12	1.60	0.83
1:D:165:ASP:OD1	5:D:502:HOH:O	1.96	0.83
1:C:311:GLU:OE1	5:C:502:HOH:O	1.99	0.79
1:A:194:ASP:HA	1:A:234:VAL:CG1	2.12	0.79
1:D:330:GLN:N	5:D:504:HOH:O	2.17	0.77
1:A:165:ASP:OD1	5:A:502:HOH:O	2.05	0.75
1:B:311:GLU:OE1	5:B:501:HOH:O	2.07	0.71
1:C:331:PHE:OXT	5:C:503:HOH:O	2.09	0.69
1:A:276:LEU:CD1	1:A:282:ILE:HG13	2.24	0.68
1:A:225:GLN:N	5:A:505:HOH:O	2.28	0.67
1:A:276:LEU:CD1	1:A:282:ILE:HG21	2.24	0.66
1:B:117:LYS:NZ	5:B:503:HOH:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:CB	1:A:103:GLU:HG2	2.26	0.65
1:D:99:GLN:CB	1:D:108:LEU:HD13	2.26	0.64
1:D:285:ASP:OD2	5:D:503:HOH:O	2.15	0.64
1:A:276:LEU:HD13	1:A:282:ILE:CG1	2.28	0.64
1:A:276:LEU:CD1	1:A:282:ILE:CB	2.76	0.64
1:A:276:LEU:HD13	1:A:282:ILE:HG13	1.80	0.62
1:B:103:GLU:OE2	1:B:107:ASN:ND2	2.19	0.62
3:C:403:SO4:O4	5:C:504:HOH:O	2.16	0.62
1:B:9:HIS:HD2	5:C:518:HOH:O	1.83	0.60
1:B:324:GLY:HA2	1:B:327:LYS:HE3	1.82	0.60
1:A:276:LEU:HD11	1:A:282:ILE:CG2	2.28	0.59
1:C:324:GLY:HA2	1:C:327:LYS:HE3	1.83	0.59
1:B:276:LEU:HD22	1:B:288[A]:LEU:HD11	1.85	0.58
1:A:296:GLN:NE2	5:A:504:HOH:O	2.25	0.58
1:A:276:LEU:HD21	1:A:288:LEU:CD1	2.32	0.58
2:C:401:NAI:C6N	4:C:402:OAA:O2	2.51	0.57
1:D:99:GLN:CB	1:D:108:LEU:HD22	2.35	0.56
1:A:276:LEU:CD1	1:A:282:ILE:HB	2.36	0.56
1:C:324:GLY:O	1:C:327:LYS:HG2	2.06	0.55
1:A:276:LEU:CD2	1:A:288:LEU:HD12	2.36	0.55
1:C:284:GLU:N	1:C:284:GLU:OE2	2.40	0.55
1:B:25:VAL:HG22	1:B:50:VAL:CG2	2.36	0.54
1:A:276:LEU:CD1	1:A:282:ILE:CG1	2.83	0.54
1:A:222:ASP:CG	1:A:224:GLU:O	2.50	0.54
1:A:25:VAL:HG13	1:A:50:VAL:HG23	1.91	0.53
1:A:276:LEU:HD21	1:A:288:LEU:HB2	1.89	0.53
1:A:276:LEU:CD1	1:A:282:ILE:CG2	2.87	0.53
1:B:9:HIS:HB2	1:C:304:LYS:HD2	1.90	0.52
1:A:276:LEU:HD11	1:A:282:ILE:HG13	1.92	0.52
1:D:318:SER:O	1:D:322:LEU:HD23	2.10	0.51
1:A:239:GLU:OE1	1:A:242:LYS:NZ	2.38	0.50
1:B:154:LYS:NZ	5:B:507:HOH:O	2.44	0.50
1:B:72:ARG:NE	5:B:502:HOH:O	2.19	0.50
1:D:225:GLN:HA	5:D:507:HOH:O	2.13	0.49
1:C:141:ILE:HD13	1:C:325:ILE:HG21	1.95	0.49
1:A:276:LEU:C	1:A:276:LEU:HD12	2.38	0.48
1:B:276:LEU:HD22	1:B:288[A]:LEU:CD1	2.42	0.48
1:B:25:VAL:HG22	1:B:50:VAL:HG21	1.95	0.48
1:C:330:GLN:O	1:C:330:GLN:HG3	2.13	0.48
1:B:276:LEU:O	1:B:276:LEU:HG	2.13	0.48
1:A:25:VAL:HG22	1:A:50:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:O	1:D:111:ARG:NH1	2.46	0.48
1:B:276:LEU:CD2	1:B:288[A]:LEU:HD11	2.43	0.48
1:C:204:ASN:HA	1:C:210:LEU:HD13	1.96	0.47
1:B:11:LEU:HD11	1:C:302:VAL:HG23	1.96	0.47
1:A:80:LYS:NZ	5:A:503:HOH:O	2.22	0.47
1:C:237:ALA:HB1	4:C:402:OAA:H22	1.97	0.47
1:A:302:VAL:HG23	1:D:11:LEU:HD11	1.97	0.46
1:A:225:GLN:HB3	1:A:228:GLN:HG2	1.98	0.46
1:A:211:LYS:NZ	1:A:217:LEU:O	2.43	0.45
1:D:99:GLN:CB	1:D:108:LEU:CD1	2.93	0.45
1:B:6:GLN:O	1:C:304:LYS:HE2	2.16	0.45
1:A:276:LEU:HD21	1:A:288:LEU:CG	2.46	0.45
1:A:100:GLN:C	1:A:103:GLU:HG2	2.41	0.45
1:A:52:VAL:O	1:A:80:LYS:HE2	2.16	0.45
1:B:25:VAL:HG13	1:B:50:VAL:HG23	1.99	0.44
1:B:107:ASN:HA	5:B:537:HOH:O	2.16	0.44
1:C:32:MET:HE1	1:C:64:LEU:HD11	1.99	0.44
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.52	0.44
1:A:168:ARG:HD3	1:A:236:SER:OG	2.18	0.44
1:B:324:GLY:HA2	1:B:327:LYS:CE	2.46	0.43
1:D:290:VAL:CG2	1:D:291:PRO:HD2	2.48	0.43
1:B:12:LEU:HD21	1:C:155:ASN:CG	2.43	0.43
1:B:179:VAL:CG1	1:B:183:SER:HB2	2.49	0.43
1:A:276:LEU:O	1:A:277:LYS:C	2.61	0.43
1:B:109:VAL:HG13	1:B:110:GLN:N	2.34	0.42
1:D:191:GLU:CG	1:D:322:LEU:HD21	2.49	0.42
1:D:290:VAL:CG2	1:D:291:PRO:CD	2.97	0.42
1:B:291:PRO:HB2	1:B:303:VAL:HB	2.01	0.42
1:B:25:VAL:HA	1:B:50:VAL:CG2	2.50	0.42
1:C:304:LYS:NZ	5:C:518:HOH:O	2.53	0.42
1:C:306:THR:OG1	5:C:506:HOH:O	2.21	0.42
1:D:110:GLN:NE2	5:D:504:HOH:O	2.37	0.42
1:B:211:LYS:HE3	5:B:658:HOH:O	2.19	0.41
1:D:329:LEU:HA	5:D:504:HOH:O	2.20	0.41
1:C:291:PRO:HB2	1:C:303:VAL:HB	2.02	0.41
1:D:191:GLU:CD	1:D:322:LEU:HD21	2.46	0.41
1:D:109:VAL:O	1:D:113:VAL:HG23	2.21	0.41
1:B:267:ARG:NH1	1:C:14:GLU:OE2	2.52	0.41
1:D:244:LYS:HE2	1:D:246:TYR:O	2.20	0.41
1:B:301:ASP:OD2	1:C:10:ASN:HA	2.21	0.40
1:C:28:GLY:HA3	2:C:401:NAI:O5B	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:GLY:HA2	1:D:327:LYS:HE3	2.03	0.40
1:D:222:ASP:O	1:D:225:GLN:NE2	2.54	0.40
1:A:239:GLU:OE1	1:A:242:LYS:HE3	2.22	0.40

All (3) 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)
5:A:660:HOH:O	5:B:641:HOH:O[1_554]	1.88	0.32
5:B:624:HOH:O	5:C:656:HOH:O[2_556]	1.96	0.24
5:A:657:HOH:O	5:D:541:HOH:O[2_656]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	267/285 (94%)	264 (99%)	3 (1%)	65	56
1	B	107/285 (38%)	106 (99%)	1 (1%)	70	63
1	C	153/285 (54%)	151 (99%)	2 (1%)	61	50
1	D	279/285 (98%)	276 (99%)	3 (1%)	65	56
All	All	806/1140 (71%)	797 (99%)	9 (1%)	65	56

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG

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Mol	Chain	Res	Type
1	A	131	LYS
1	A	227	LYS
1	B	331	PHE
1	C	227	LYS
1	C	276	LEU
1	D	104	SER
1	D	276	LEU
1	D	316	LYS

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

Mol	Chain	Res	Type
1	A	9	HIS
1	A	20	ASN
1	A	122	ASN
1	A	232	GLN
1	D	20	ASN
1	D	137	ASN
1	D	326	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	B	401	-	47,48,48	3.45	22 (46%)	64,73,73	1.87	18 (28%)
3	SO4	C	403	-	4,4,4	0.49	0	6,6,6	0.15	0
2	NAI	D	401	-	47,48,48	3.69	22 (46%)	64,73,73	2.12	18 (28%)
4	OAA	D	402	-	8,8,8	2.55	3 (37%)	8,10,10	1.87	2 (25%)
4	OAA	C	402	-	8,8,8	2.32	3 (37%)	8,10,10	2.04	3 (37%)
2	NAI	C	401	-	47,48,48	3.26	20 (42%)	64,73,73	1.93	19 (29%)
2	NAI	A	401	-	47,48,48	3.65	23 (48%)	64,73,73	1.94	18 (28%)
3	SO4	A	402	-	4,4,4	0.55	0	6,6,6	0.27	0
3	SO4	D	403	-	4,4,4	0.46	0	6,6,6	0.38	0
3	SO4	B	402	-	4,4,4	0.31	0	6,6,6	0.42	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	B	401	-	-	5/29/72/72	0/5/5/5
2	NAI	D	401	-	-	5/29/72/72	0/5/5/5
4	OAA	D	402	-	-	2/8/8/8	-
4	OAA	C	402	-	-	4/8/8/8	-
2	NAI	C	401	-	-	5/29/72/72	0/5/5/5
2	NAI	A	401	-	-	7/29/72/72	0/5/5/5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAI	C2D-C1D	-8.62	1.26	1.53
2	A	401	NAI	C2D-C1D	-8.52	1.26	1.53
2	A	401	NAI	O4D-C1D	8.40	1.61	1.42
2	B	401	NAI	C2D-C1D	-8.16	1.27	1.53
2	A	401	NAI	C2B-C1B	-7.88	1.28	1.53
2	D	401	NAI	O4D-C1D	7.85	1.60	1.42
2	D	401	NAI	O4B-C1B	7.78	1.60	1.42
2	C	401	NAI	C2D-C1D	-7.66	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C2B-C1B	-7.64	1.29	1.53
2	D	401	NAI	C2B-C1B	-7.63	1.29	1.53
2	A	401	NAI	O4B-C1B	7.40	1.59	1.42
2	C	401	NAI	C2B-C1B	-7.17	1.31	1.53
2	B	401	NAI	O4D-C1D	7.13	1.58	1.42
2	A	401	NAI	C2N-C3N	7.01	1.54	1.35
2	B	401	NAI	C2N-C3N	6.94	1.54	1.35
2	D	401	NAI	C2N-C3N	6.71	1.53	1.35
2	C	401	NAI	C2N-C3N	6.63	1.53	1.35
2	C	401	NAI	O4D-C1D	6.60	1.57	1.42
2	B	401	NAI	C6N-C5N	6.43	1.52	1.33
2	C	401	NAI	C6N-C5N	6.30	1.52	1.33
2	C	401	NAI	O4B-C1B	6.29	1.56	1.42
2	A	401	NAI	C6N-C5N	6.08	1.51	1.33
2	A	401	NAI	O4B-C4B	-5.95	1.31	1.45
2	D	401	NAI	O4B-C4B	-5.93	1.31	1.45
2	D	401	NAI	C6N-C5N	5.92	1.51	1.33
2	B	401	NAI	O4B-C1B	5.89	1.55	1.42
2	C	401	NAI	O4B-C4B	-5.72	1.32	1.45
2	D	401	NAI	PN-O3	5.59	1.65	1.59
2	A	401	NAI	PN-O3	5.57	1.65	1.59
2	D	401	NAI	O4D-C4D	-5.45	1.32	1.45
2	D	401	NAI	PA-O3	5.30	1.65	1.59
2	A	401	NAI	O4D-C4D	-5.28	1.33	1.45
2	B	401	NAI	O4B-C4B	-5.25	1.33	1.45
2	C	401	NAI	PN-O3	5.20	1.65	1.59
4	D	402	OAA	O3-C3	5.04	1.33	1.23
2	D	401	NAI	O2B-C2B	5.02	1.55	1.43
2	B	401	NAI	C7N-N7N	4.97	1.47	1.33
2	A	401	NAI	C6A-N6A	4.96	1.46	1.34
2	D	401	NAI	C7N-N7N	4.93	1.47	1.33
2	B	401	NAI	C6A-N6A	4.88	1.46	1.34
2	B	401	NAI	O4D-C4D	-4.87	1.34	1.45
2	D	401	NAI	C6A-N6A	4.77	1.46	1.34
2	B	401	NAI	PN-O3	4.76	1.64	1.59
2	A	401	NAI	C7N-N7N	4.68	1.46	1.33
2	C	401	NAI	C7N-N7N	4.66	1.46	1.33
2	C	401	NAI	O4D-C4D	-4.63	1.34	1.45
4	C	402	OAA	O3-C3	4.30	1.31	1.23
2	C	401	NAI	C6A-N6A	4.25	1.45	1.34
2	A	401	NAI	O2B-C2B	4.24	1.53	1.43
2	A	401	NAI	PA-O3	4.24	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	OAA	O4-C4	4.06	1.32	1.22
2	B	401	NAI	PA-O3	3.86	1.63	1.59
2	B	401	NAI	C6N-N1N	3.84	1.46	1.37
2	B	401	NAI	O2B-C2B	3.83	1.52	1.43
2	D	401	NAI	O2D-C2D	3.77	1.52	1.43
2	C	401	NAI	O2B-C2B	3.52	1.51	1.43
2	A	401	NAI	O2D-C2D	3.39	1.51	1.43
2	C	401	NAI	C6N-N1N	3.35	1.45	1.37
2	B	401	NAI	C5B-C4B	3.29	1.61	1.51
4	C	402	OAA	O1-C1	3.27	1.32	1.22
4	C	402	OAA	O4-C4	3.13	1.30	1.22
2	A	401	NAI	C6N-N1N	3.10	1.44	1.37
2	D	401	NAI	C5D-C4D	3.09	1.60	1.51
2	A	401	NAI	C7N-C3N	3.07	1.55	1.48
2	B	401	NAI	C5D-C4D	3.07	1.60	1.51
2	D	401	NAI	C5A-C4A	-3.03	1.33	1.39
2	A	401	NAI	C5D-C4D	3.03	1.60	1.51
2	D	401	NAI	C7N-C3N	3.03	1.55	1.48
2	B	401	NAI	C7N-C3N	2.99	1.55	1.48
2	D	401	NAI	C6N-N1N	2.98	1.44	1.37
2	A	401	NAI	C5A-C4A	-2.94	1.33	1.39
2	B	401	NAI	O2D-C2D	2.93	1.50	1.43
2	B	401	NAI	C2A-N3A	2.93	1.39	1.33
4	D	402	OAA	O1-C1	2.90	1.31	1.22
2	C	401	NAI	C5D-C4D	2.83	1.60	1.51
2	C	401	NAI	C7N-C3N	2.61	1.54	1.48
2	A	401	NAI	C5B-C4B	2.61	1.59	1.51
2	D	401	NAI	C5B-C4B	2.59	1.59	1.51
2	C	401	NAI	C5A-C4A	-2.54	1.34	1.39
2	C	401	NAI	C5A-N7A	-2.49	1.34	1.39
2	C	401	NAI	C5B-C4B	2.49	1.59	1.51
2	A	401	NAI	O3D-C3D	-2.36	1.37	1.43
2	B	401	NAI	O3D-C3D	-2.33	1.37	1.43
2	A	401	NAI	PN-O5D	2.30	1.68	1.59
2	D	401	NAI	O3D-C3D	-2.29	1.37	1.43
2	B	401	NAI	C4N-C5N	2.29	1.54	1.49
2	A	401	NAI	C4N-C5N	2.25	1.54	1.49
2	D	401	NAI	O3B-C3B	-2.22	1.37	1.43
2	C	401	NAI	O2D-C2D	2.16	1.48	1.43
2	C	401	NAI	C2A-N3A	2.14	1.37	1.33
2	D	401	NAI	PN-O5D	2.13	1.67	1.59
2	A	401	NAI	C2A-N3A	2.04	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C5A-C4A	-2.03	1.35	1.39

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAI	N3A-C2A-N1A	-6.74	118.38	128.58
2	A	401	NAI	N3A-C2A-N1A	-5.88	119.69	128.58
2	C	401	NAI	N3A-C2A-N1A	-5.24	120.65	128.58
2	D	401	NAI	N6A-C6A-N1A	-4.99	107.27	118.38
2	B	401	NAI	N3A-C2A-N1A	-4.98	121.05	128.58
2	A	401	NAI	N9A-C8A-N7A	-4.81	107.11	113.94
2	D	401	NAI	N9A-C8A-N7A	-4.70	107.27	113.94
2	C	401	NAI	C5A-C4A-N3A	-4.51	120.51	126.72
2	A	401	NAI	C5A-C4A-N3A	-4.47	120.56	126.72
2	D	401	NAI	C3N-C2N-N1N	-4.47	116.65	123.20
2	D	401	NAI	C5A-C4A-N3A	-4.39	120.67	126.72
2	C	401	NAI	C4B-O4B-C1B	-4.26	100.06	109.47
2	C	401	NAI	N9A-C8A-N7A	-4.24	107.92	113.94
4	C	402	OAA	O4-C4-C3	-4.11	116.69	121.81
2	B	401	NAI	C5A-C4A-N3A	-4.07	121.12	126.72
2	D	401	NAI	O4B-C1B-N9A	4.06	115.90	108.09
2	B	401	NAI	N6A-C6A-N1A	-4.02	109.42	118.38
2	A	401	NAI	N6A-C6A-N1A	-4.00	109.46	118.38
2	B	401	NAI	N9A-C8A-N7A	-3.95	108.33	113.94
4	D	402	OAA	O3-C3-C2	3.93	126.45	120.41
2	B	401	NAI	O4B-C1B-C2B	-3.91	98.26	106.62
2	C	401	NAI	N3A-C4A-N9A	3.66	133.39	127.17
2	D	401	NAI	C2A-N3A-C4A	3.63	120.71	111.83
2	D	401	NAI	C4B-O4B-C1B	-3.60	101.51	109.47
2	A	401	NAI	C1D-N1N-C2N	-3.54	115.30	121.14
2	D	401	NAI	C5A-C6A-N6A	3.41	131.72	123.29
2	A	401	NAI	C2A-N3A-C4A	3.31	119.92	111.83
2	D	401	NAI	C1D-N1N-C2N	-3.27	115.76	121.14
2	A	401	NAI	C5A-N7A-C8A	3.14	108.38	103.45
2	B	401	NAI	C1D-N1N-C2N	-3.06	116.11	121.14
2	A	401	NAI	C4D-O4D-C1D	-3.04	102.75	109.47
2	C	401	NAI	O4B-C1B-C2B	-3.02	100.16	106.62
2	C	401	NAI	N6A-C6A-N1A	-3.00	111.69	118.38
2	D	401	NAI	C5A-N7A-C8A	2.98	108.14	103.45
2	A	401	NAI	N3A-C4A-N9A	2.97	132.22	127.17
2	A	401	NAI	C4A-N9A-C8A	2.97	108.86	105.74
4	C	402	OAA	O3-C3-C4	2.96	123.89	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAI	C4A-N9A-C8A	2.90	108.79	105.74
2	C	401	NAI	C2A-N3A-C4A	2.88	118.86	111.83
2	A	401	NAI	C5A-C6A-N6A	2.87	130.39	123.29
2	D	401	NAI	C4A-N9A-C8A	2.86	108.74	105.74
2	D	401	NAI	N3A-C4A-N9A	2.85	132.02	127.17
2	B	401	NAI	C5A-C6A-N6A	2.85	130.34	123.29
2	B	401	NAI	C4B-O4B-C1B	-2.72	103.45	109.47
2	C	401	NAI	C2B-C3B-C4B	-2.72	97.35	102.61
2	B	401	NAI	C2A-N3A-C4A	2.71	118.45	111.83
2	B	401	NAI	C4D-O4D-C1D	-2.66	103.58	109.47
2	B	401	NAI	C4A-N9A-C8A	2.66	108.53	105.74
2	A	401	NAI	C5D-C4D-C3D	-2.65	105.66	115.21
2	C	401	NAI	O4B-C4B-C3B	2.62	110.34	105.15
2	A	401	NAI	O1N-PN-O3	2.60	114.30	107.27
4	C	402	OAA	O5-C4-C3	2.57	120.73	113.59
2	B	401	NAI	N3A-C4A-N9A	2.55	131.50	127.17
2	B	401	NAI	O2A-PA-O3	2.55	114.16	107.27
2	B	401	NAI	C2B-C3B-C4B	-2.54	97.69	102.61
2	D	401	NAI	C4A-N9A-C1B	-2.54	120.70	126.63
2	C	401	NAI	C6N-N1N-C2N	2.47	121.96	119.32
2	D	401	NAI	C5B-C4B-C3B	-2.44	106.44	115.21
4	D	402	OAA	O2-C1-C2	2.43	122.05	114.51
2	B	401	NAI	C3B-C2B-C1B	2.34	105.89	101.46
2	A	401	NAI	C4B-O4B-C1B	-2.33	104.33	109.47
2	C	401	NAI	C4D-O4D-C1D	-2.33	104.33	109.47
2	A	401	NAI	O4B-C1B-N9A	2.33	112.56	108.09
2	C	401	NAI	O3B-C3B-C4B	2.33	117.77	111.08
2	D	401	NAI	O5B-C5B-C4B	-2.32	101.08	108.99
2	D	401	NAI	O4B-C4B-C3B	2.30	109.72	105.15
2	C	401	NAI	O4B-C4B-C5B	-2.28	102.05	109.33
2	C	401	NAI	C3N-C2N-N1N	-2.27	119.87	123.20
2	C	401	NAI	C1D-N1N-C2N	-2.22	117.47	121.14
2	A	401	NAI	C4A-N9A-C1B	-2.22	121.44	126.63
2	C	401	NAI	O3D-C3D-C2D	-2.19	104.80	111.82
2	C	401	NAI	O3-PA-O1A	-2.16	104.20	110.70
2	D	401	NAI	C4D-O4D-C1D	-2.15	104.71	109.47
2	B	401	NAI	O4B-C1B-N9A	2.14	112.21	108.09
2	A	401	NAI	O5B-C5B-C4B	-2.12	101.78	108.99
2	A	401	NAI	C5B-C4B-C3B	-2.11	107.63	115.21
2	B	401	NAI	C3N-C2N-N1N	-2.09	120.13	123.20
2	B	401	NAI	C5D-C4D-C3D	-2.02	107.94	115.21

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C2D-C1D-N1N-C6N
4	C	402	OAA	O3-C3-C4-O5
4	C	402	OAA	C2-C3-C4-O4
4	C	402	OAA	C2-C3-C4-O5
4	D	402	OAA	C2-C3-C4-O5
2	B	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C6N
4	C	402	OAA	O3-C3-C4-O4
2	B	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	C5B-O5B-PA-O1A
2	C	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	C2N-C3N-C7N-N7N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	C2B-C1B-N9A-C8A
4	D	402	OAA	O1-C1-C2-C3
2	C	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	C2B-C1B-N9A-C8A
2	A	401	NAI	O4B-C4B-C5B-O5B

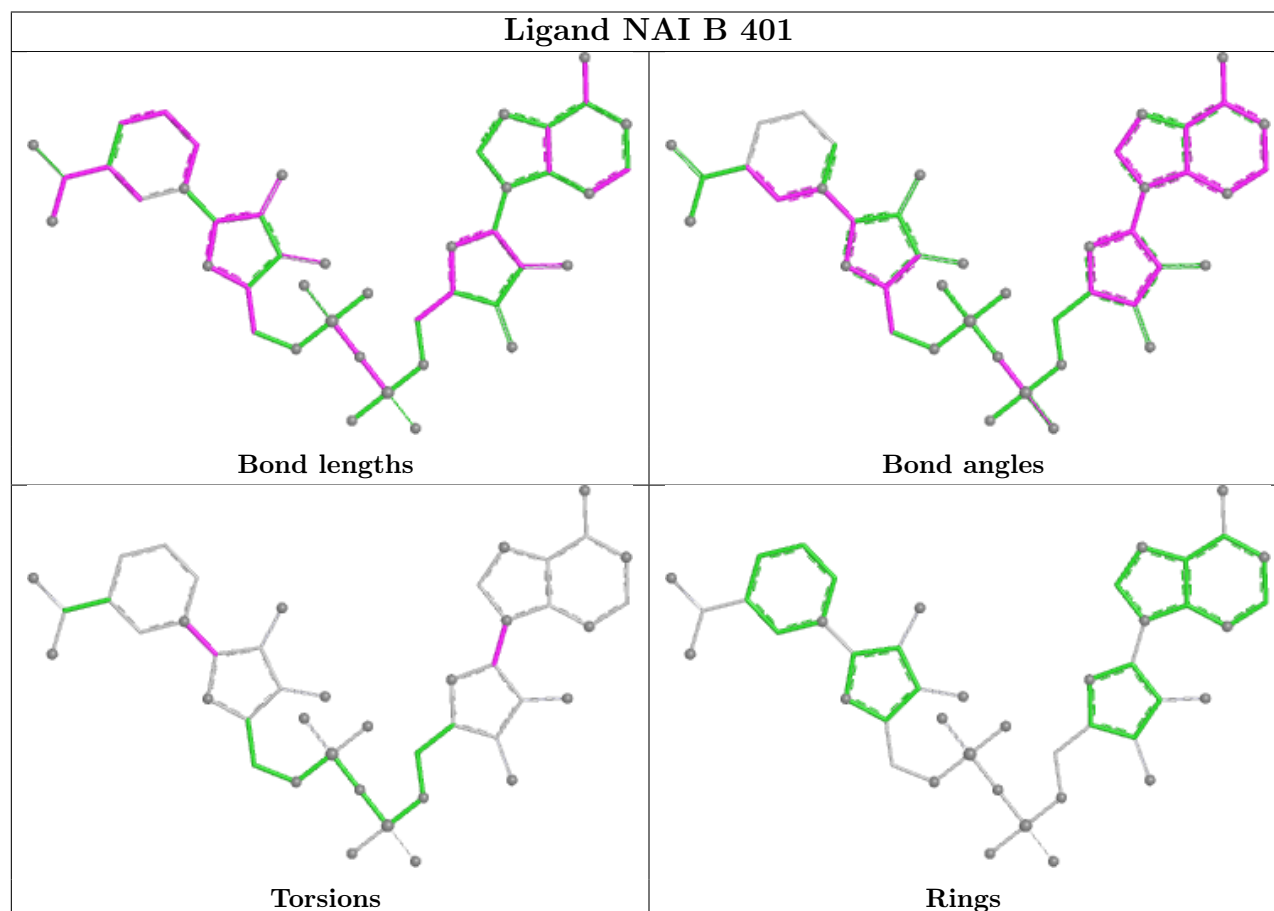
There are no ring outliers.

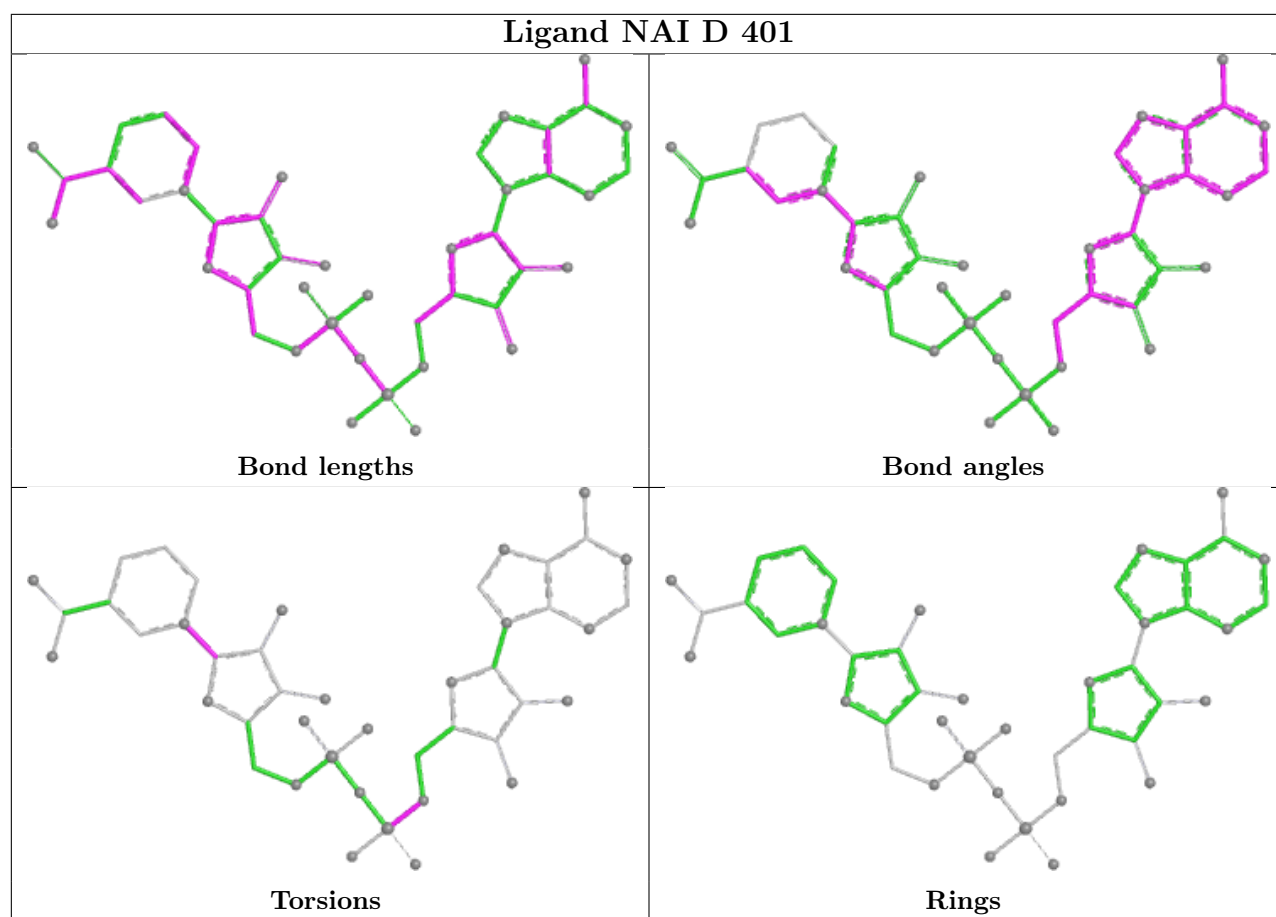
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	SO4	1	0
4	C	402	OAA	2	0
2	C	401	NAI	2	0

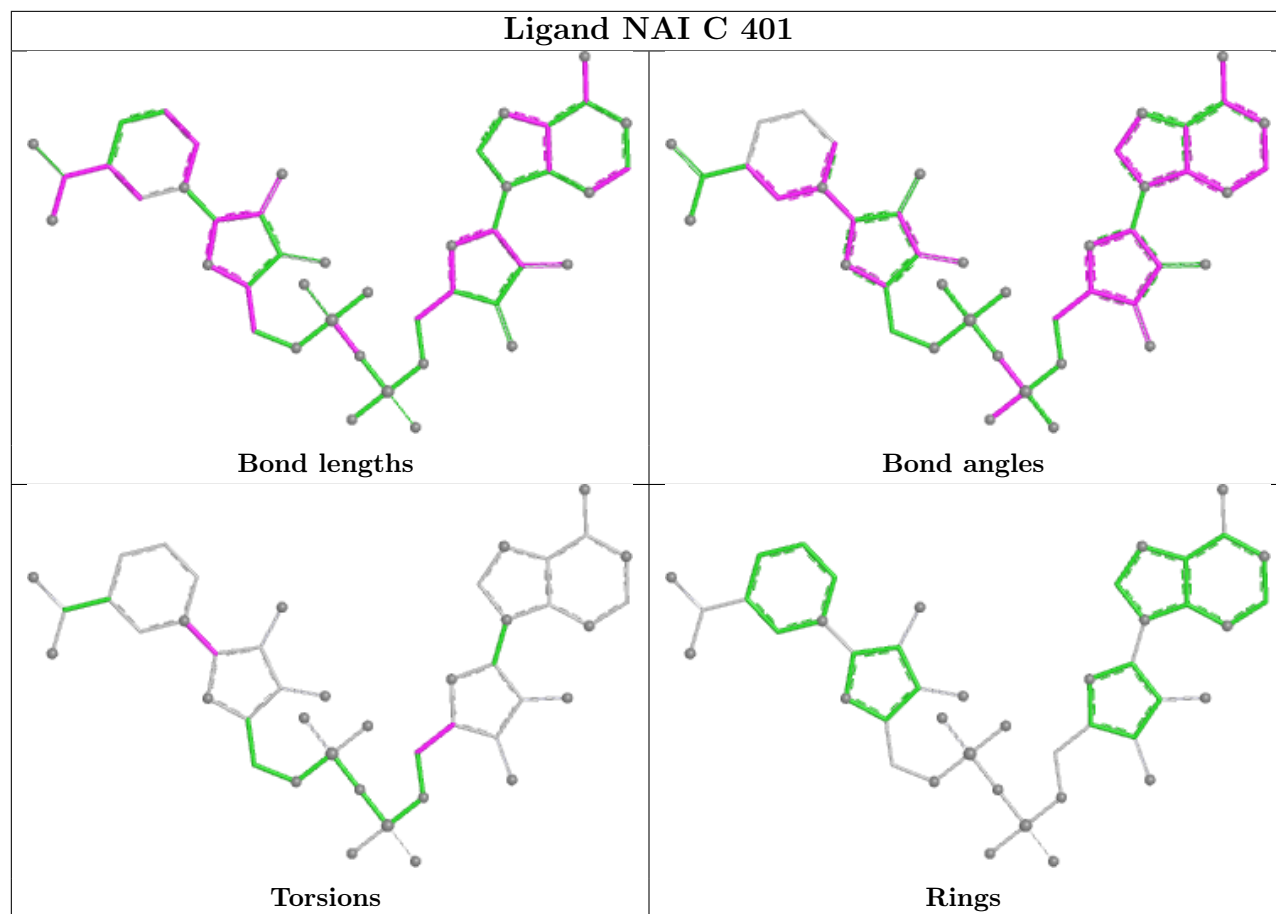
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

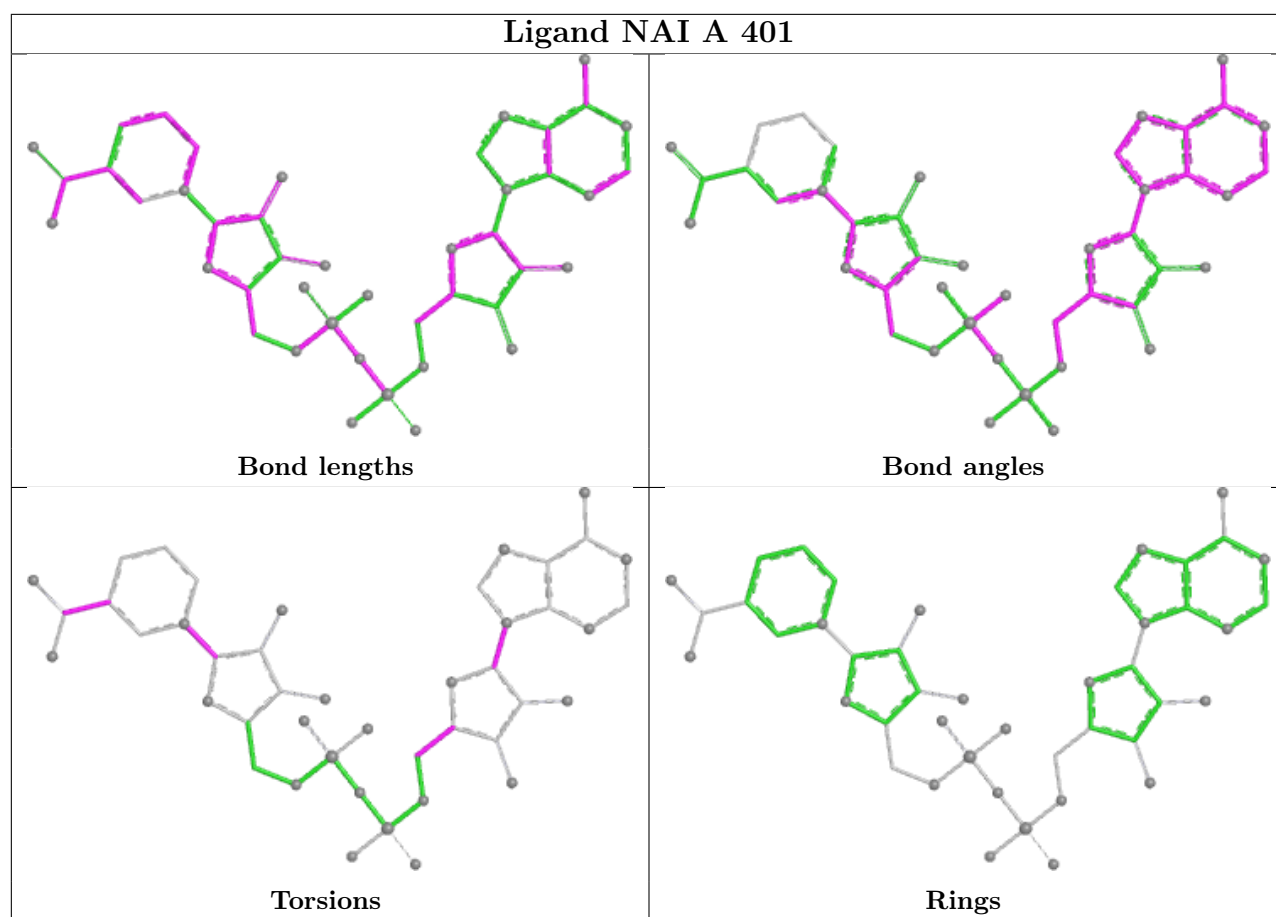
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand NAI C 401





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	331/332 (99%)	0.10	19 (5%)	29 31	18, 31, 78, 118	1 (0%)
1	B	331/332 (99%)	-0.01	9 (2%)	56 61	19, 31, 62, 99	2 (0%)
1	C	331/332 (99%)	-0.08	10 (3%)	52 57	17, 30, 59, 95	2 (0%)
1	D	331/332 (99%)	0.04	16 (4%)	35 37	17, 30, 71, 113	3 (0%)
All	All	1324/1328 (99%)	0.01	54 (4%)	41 45	17, 31, 66, 118	8 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	331	PHE	8.0
1	A	331	PHE	7.5
1	A	276	LEU	5.1
1	A	99	GLN	4.6
1	D	221	ALA	4.1
1	D	100	GLN	4.1
1	C	14	GLU	3.7
1	D	14	GLU	3.6
1	A	108	LEU	3.3
1	B	331	PHE	3.1
1	B	16	HIS	3.0
1	C	323	TRP	3.0
1	D	101	GLU	3.0
1	A	329	LEU	2.9
1	D	226	TRP	2.9
1	B	100	GLN	2.9
1	D	106	LEU	2.9
1	D	330	GLN	2.9
1	C	1	ALA	2.8
1	C	16	HIS	2.8
1	D	15	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	330	GLN	2.7
1	D	102	GLY	2.6
1	A	101	GLU	2.6
1	A	221	ALA	2.6
1	A	234	VAL	2.4
1	D	329	LEU	2.4
1	A	15	GLU	2.4
1	A	213	LEU	2.4
1	A	103	GLU	2.4
1	C	331	PHE	2.3
1	A	328	GLU	2.3
1	A	100	GLN	2.3
1	D	97	ALA	2.3
1	A	105	ARG	2.3
1	D	238	TYR	2.3
1	A	106	LEU	2.3
1	D	319	ALA	2.3
1	D	98	ARG	2.3
1	C	320	ASP	2.2
1	C	322	LEU	2.2
1	A	97	ALA	2.2
1	B	13	LYS	2.2
1	B	103	GLU	2.2
1	A	1	ALA	2.2
1	B	1	ALA	2.2
1	C	221	ALA	2.2
1	B	14	GLU	2.1
1	A	323	TRP	2.1
1	B	107	ASN	2.1
1	D	11	LEU	2.1
1	A	214	HIS	2.0
1	B	102	GLY	2.0
1	C	319	ALA	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 ⓘ

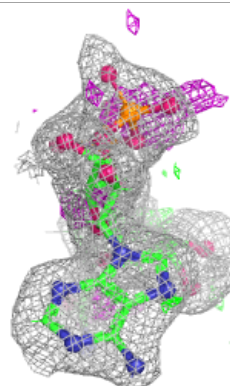
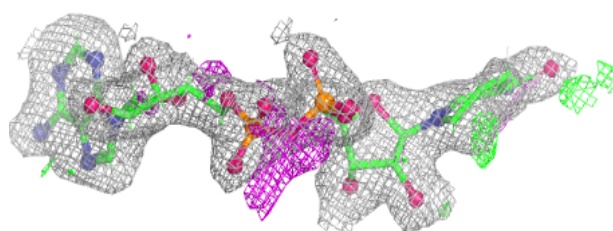
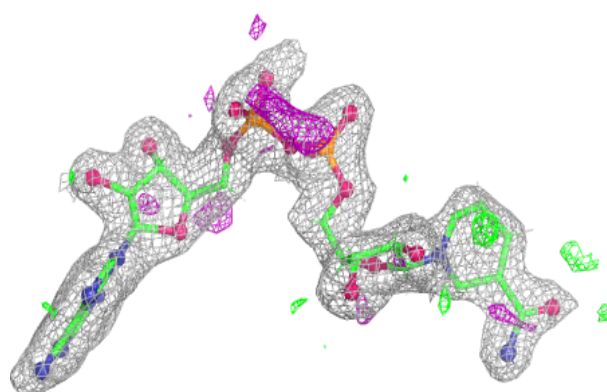
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OAA	D	402	9/9	0.77	0.19	32,42,52,56	11
4	OAA	C	402	9/9	0.84	0.18	24,29,34,36	11
2	NAI	D	401	44/44	0.92	0.09	26,40,50,58	0
3	SO4	B	402	5/5	0.92	0.15	34,38,42,47	0
3	SO4	A	402	5/5	0.93	0.16	31,36,37,42	0
2	NAI	A	401	44/44	0.95	0.08	25,37,54,58	0
3	SO4	D	403	5/5	0.95	0.15	28,29,41,44	0
3	SO4	C	403	5/5	0.96	0.13	32,34,42,44	0
2	NAI	C	401	44/44	0.98	0.06	19,26,35,42	0
2	NAI	B	401	44/44	0.98	0.06	16,25,43,51	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.

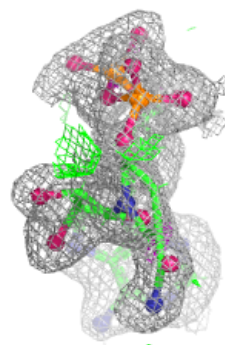
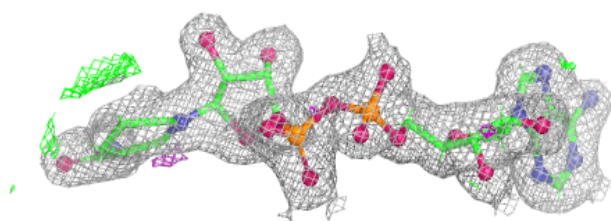
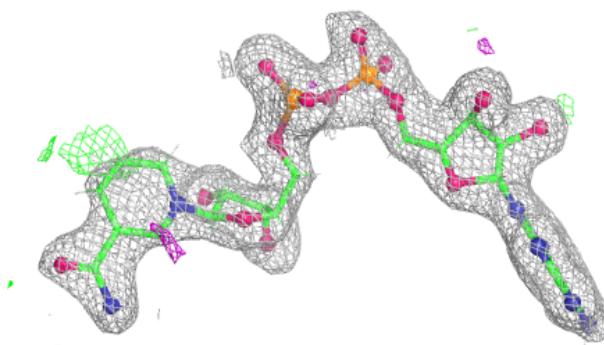
Electron density around NAI D 401:

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

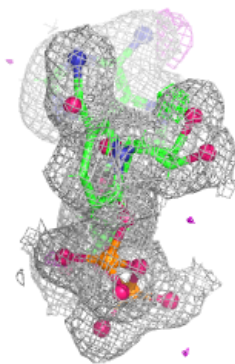
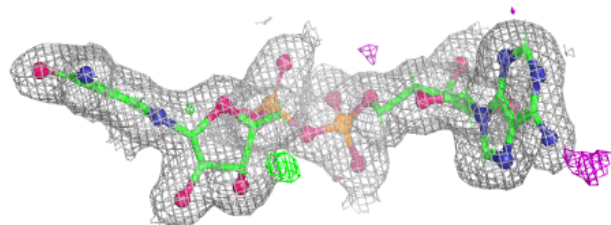
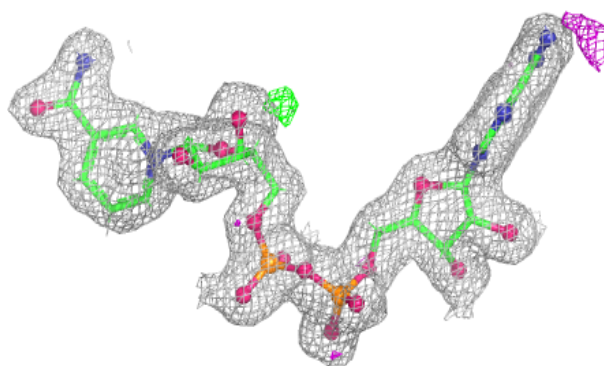


Electron density around NAI A 401:

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

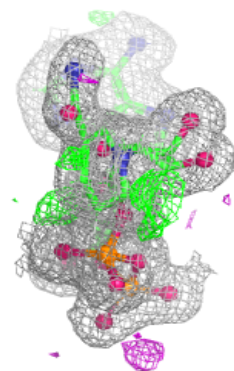
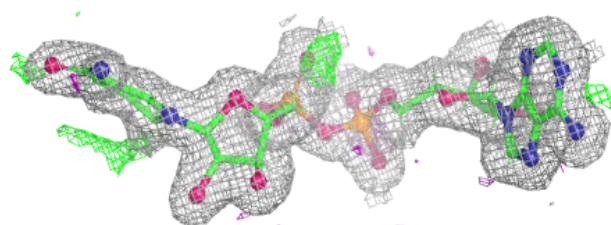
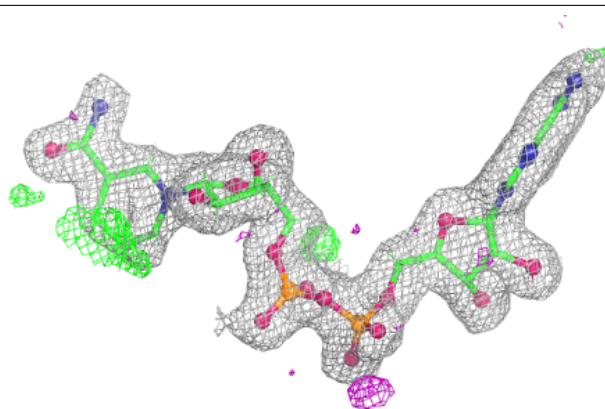
**Electron density around NAI C 401:**

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



Electron density around NAI 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.