Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 05:35 am BST

PDB ID	:	5NQQ
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 (i) symbol.

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

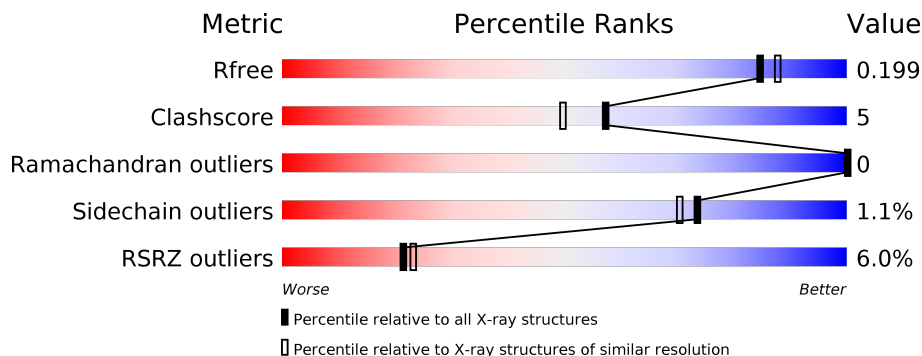|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.87 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	Percentile Ranks	Value
Rfree		0.199
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		6.0%

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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	332	8% 91% 8% •
1	B	332	6% 91% 8% •
1	C	332	5% 92% 7%
1	D	332	6% 92% 8%

2 Entry composition (i)

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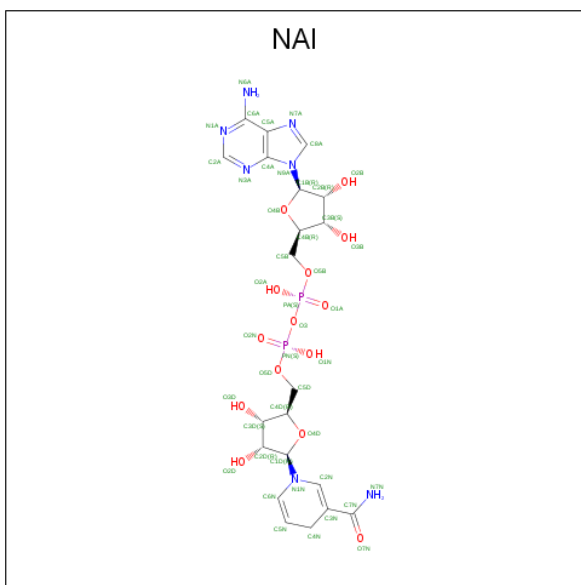
- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

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 (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
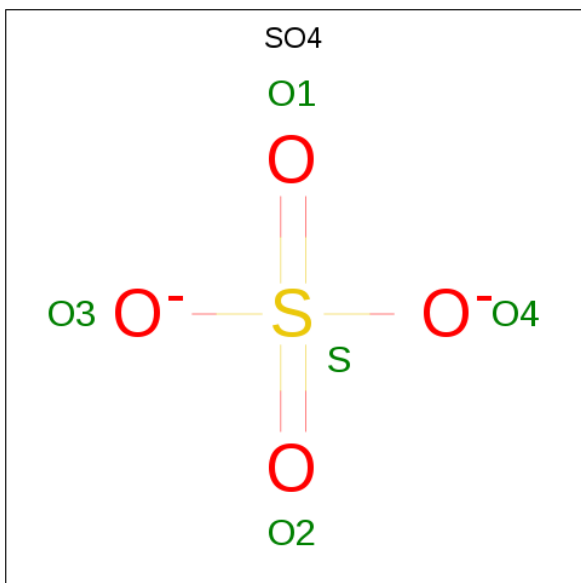
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

- Molecule 4 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).
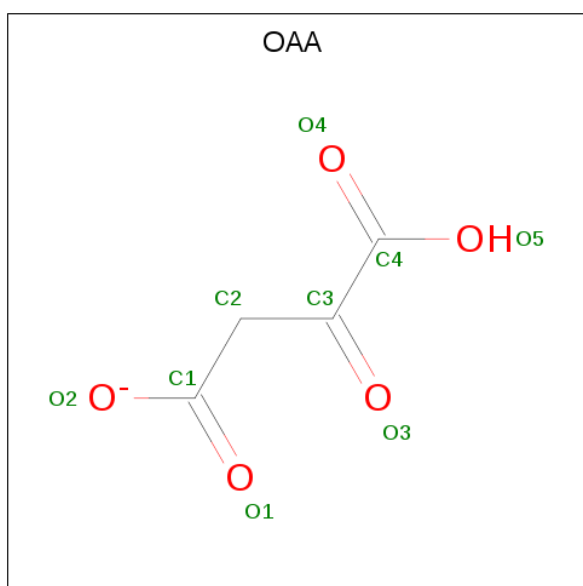
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 11	C 4	H 2	O 5	0	0
4	D	1	Total 11	C 4	H 2	O 5	0	0

- Molecule 5 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
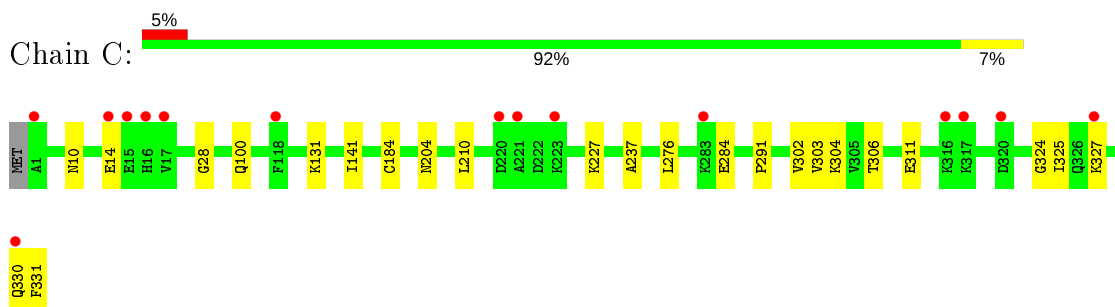
- Molecule 1: L-lactate dehydrogenase A chain
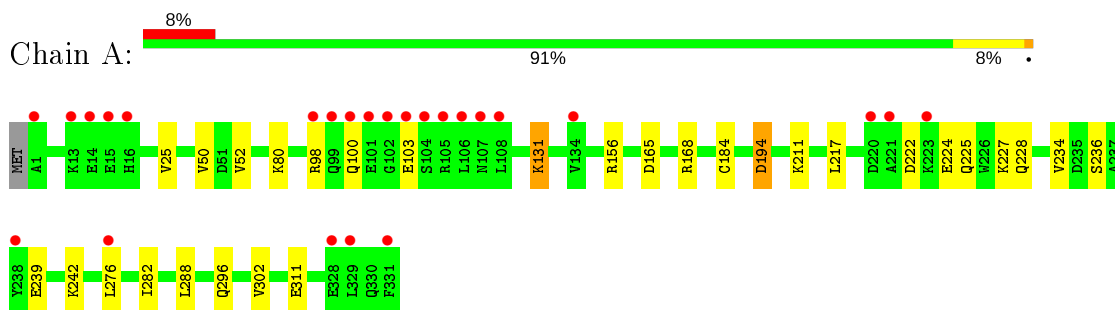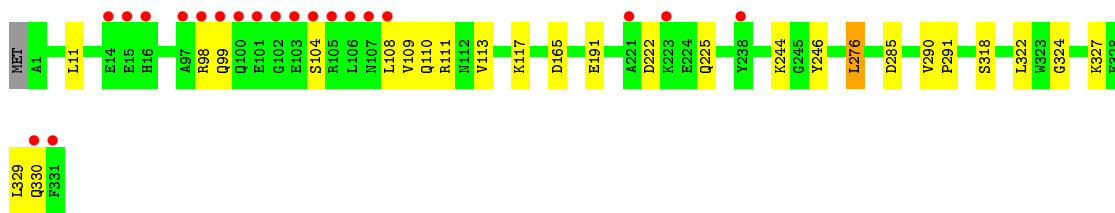

- Molecule 1: L-lactate dehydrogenase A chain
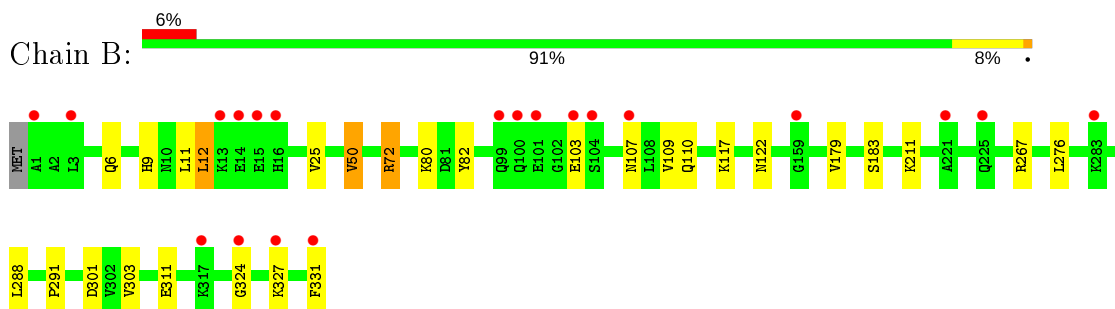
- Molecule 1: L-lactate dehydrogenase A chain

- Molecule 1: L-lactate dehydrogenase A chain

4 Data and refinement statistics (i)

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) 98.9 (29.42-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.87Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.170 , 0.199 0.171 , 0.199	Depositor DCC
R_{free} test set	5627 reflections (5.02%)	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 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	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.*

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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: NAI, SO4, OAA

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	0.54	1/2595 (0.0%)	0.67	1/3510 (0.0%)
1	B	0.55	1/2603 (0.0%)	0.72	2/3521 (0.1%)
1	C	0.54	1/2624 (0.0%)	0.65	0/3546
1	D	0.54	0/2596	0.69	1/3513 (0.0%)
All	All	0.54	3/10418 (0.0%)	0.68	4/14090 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	CYS	CB-SG	-6.87	1.70	1.82
1	C	184	CYS	CB-SG	-5.38	1.73	1.81
1	B	50	VAL	CB-CG2	-5.08	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	LEU	CA-CB-CG	7.12	131.68	115.30
1	D	276	LEU	CB-CG-CD2	-6.57	99.84	111.00
1	A	156	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	B	72	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	26	0
1	C	2569	2654	2655	19	0
1	D	2539	2614	2616	20	0
2	A	44	27	26	0	0
2	B	44	27	27	0	0
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	6	2
5	B	184	0	0	5	2
5	C	203	0	0	7	1
5	D	185	0	0	7	1
All	All	11166	10620	10626	102	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 (102) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:117:LYS:NZ	5:B:503:HOH:O	2.27	0.66
1:A:276:LEU:CD1	1:A:282:ILE:HG21	2.24	0.66
1:A:100:GLN:CB	1:A:103:GLU:HG2	2.26	0.65
1:D:285:ASP:OD2	5:D:503:HOH:O	2.15	0.64
1:D:99:GLN:CB	1:D:108:LEU:HD13	2.26	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:A:131:LYS:NZ	5:A:507:HOH:O	2.35	0.58
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:OE2	1:C:284:GLU:N	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: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:A:80:LYS:NZ	5:A:503:HOH:O	2.22	0.51
1:D:117:LYS:NZ	5:D:501:HOH:O	1.92	0.51
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:72:ARG:NE	5:B:502:HOH:O	2.19	0.50
1:A:222:ASP:CG	1:A:224:GLU:O	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG	1:B:276:LEU:O	2.13	0.48
1:A:25:VAL:HG22	1:A:50:VAL:CG2	2.44	0.48
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: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: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: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:A:276:LEU:C	1:A:276:LEU:HD12	2.38	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:179:VAL:CG1	1:B:183:SER:HB2	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:324:GLY:HA2	1:D:327:LYS:HE3	2.03	0.40
1:A:100:GLN:C	1:A:103:GLU:HG2	2.41	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)

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	330/332 (99%)	324 (98%)	6 (2%)	0	100	100
1	B	331/332 (100%)	325 (98%)	6 (2%)	0	100	100
1	C	331/332 (100%)	325 (98%)	6 (2%)	0	100	100
1	D	332/332 (100%)	326 (98%)	6 (2%)	0	100	100
All	All	1324/1328 (100%)	1300 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	281/285 (99%)	277 (99%)	4 (1%)	67	62
1	B	282/285 (99%)	278 (99%)	4 (1%)	67	62
1	C	286/285 (100%)	283 (99%)	3 (1%)	76	73
1	D	279/285 (98%)	277 (99%)	2 (1%)	84	83
All	All	1128/1140 (99%)	1115 (99%)	13 (1%)	73	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	A	131	LYS
1	A	194	ASP
1	A	227	LYS
1	B	12	LEU
1	B	80[A]	LYS
1	B	80[B]	LYS
1	B	331	PHE
1	C	131	LYS
1	C	227	LYS
1	C	276	LEU
1	D	104	SER
1	D	276	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	$\#|Z| > 2$
3	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.46	0
2	NAI	D	401	-	42,48,48	4.76	21 (50%)	47,73,73	2.17	11 (23%)
2	NAI	B	401	-	42,48,48	4.53	20 (47%)	47,73,73	2.07	11 (23%)
4	OAA	D	402	-	2,8,8	5.02	1 (50%)	2,10,10	2.82	1 (50%)
3	SO4	C	403	-	4,4,4	0.40	0	6,6,6	0.18	0
2	NAI	C	401	-	42,48,48	4.34	18 (42%)	47,73,73	1.86	13 (27%)
3	SO4	A	402	-	4,4,4	0.47	0	6,6,6	0.26	0
2	NAI	A	401	-	42,48,48	4.77	21 (50%)	47,73,73	1.97	11 (23%)
3	SO4	D	403	-	4,4,4	0.40	0	6,6,6	0.39	0
4	OAA	C	402	-	2,8,8	4.32	1 (50%)	2,10,10	1.99	1 (50%)

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	D	401	-	-	6/25/72/72	0/5/5/5
2	NAI	B	401	-	-	5/25/72/72	0/5/5/5
4	OAA	D	402	-	-	0/2/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OAA	C	402	-	-	2/2/8/8	-
2	NAI	C	401	-	-	5/25/72/72	0/5/5/5
2	NAI	A	401	-	-	6/25/72/72	0/5/5/5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C2B-C1B	-16.50	1.28	1.53
2	B	401	NAI	C2B-C1B	-16.00	1.29	1.53
2	D	401	NAI	C2B-C1B	-15.99	1.29	1.53
2	C	401	NAI	C2B-C1B	-15.03	1.31	1.53
2	D	401	NAI	O4B-C1B	13.54	1.60	1.41
2	A	401	NAI	O4B-C1B	12.92	1.59	1.41
2	C	401	NAI	O4B-C1B	11.07	1.56	1.41
2	B	401	NAI	C6N-C5N	10.95	1.52	1.33
2	C	401	NAI	C6N-C5N	10.73	1.52	1.33
2	B	401	NAI	O4B-C1B	10.42	1.55	1.41
2	A	401	NAI	C6N-C5N	10.34	1.51	1.33
2	D	401	NAI	C6N-C5N	10.07	1.51	1.33
2	D	401	NAI	C2D-C1D	-8.47	1.26	1.53
2	A	401	NAI	C2D-C1D	-8.37	1.26	1.53
2	A	401	NAI	O4D-C1D	8.19	1.61	1.42
2	B	401	NAI	C2D-C1D	-8.02	1.27	1.53
2	D	401	NAI	O4D-C1D	7.66	1.60	1.42
2	C	401	NAI	C2D-C1D	-7.52	1.29	1.53
2	A	401	NAI	C2N-C3N	6.98	1.54	1.34
2	B	401	NAI	O4D-C1D	6.95	1.58	1.42
2	B	401	NAI	C2N-C3N	6.91	1.54	1.34
4	D	402	OAA	O3-C3	6.88	1.33	1.22
2	D	401	NAI	C2N-C3N	6.68	1.53	1.34
2	C	401	NAI	C2N-C3N	6.60	1.53	1.34
2	C	401	NAI	O4D-C1D	6.44	1.57	1.42
4	C	402	OAA	O3-C3	5.95	1.31	1.22
2	A	401	NAI	O4B-C4B	-5.93	1.31	1.45
2	D	401	NAI	O4B-C4B	-5.90	1.31	1.45
2	C	401	NAI	O4B-C4B	-5.69	1.32	1.45
2	D	401	NAI	O4D-C4D	-5.42	1.32	1.45
2	B	401	NAI	C7N-N7N	5.39	1.47	1.33
2	D	401	NAI	C7N-N7N	5.35	1.47	1.33
2	D	401	NAI	O2B-C2B	5.26	1.55	1.43
2	A	401	NAI	O4D-C4D	-5.25	1.33	1.45
2	B	401	NAI	O4B-C4B	-5.22	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C7N-N7N	5.08	1.46	1.33
2	C	401	NAI	C7N-N7N	5.05	1.46	1.33
2	B	401	NAI	O4D-C4D	-4.85	1.34	1.45
2	C	401	NAI	O4D-C4D	-4.61	1.34	1.45
2	A	401	NAI	O2B-C2B	4.45	1.53	1.43
2	B	401	NAI	C2A-N3A	4.36	1.39	1.32
2	B	401	NAI	O2B-C2B	4.02	1.52	1.43
2	D	401	NAI	O2D-C2D	3.96	1.52	1.43
2	B	401	NAI	C6N-N1N	3.72	1.46	1.37
2	C	401	NAI	O2B-C2B	3.69	1.51	1.43
2	A	401	NAI	O2D-C2D	3.56	1.51	1.43
2	A	401	NAI	C6A-N6A	3.52	1.46	1.34
2	C	401	NAI	C2A-N3A	3.50	1.37	1.32
2	B	401	NAI	C6A-N6A	3.46	1.46	1.34
2	A	401	NAI	C2A-N3A	3.39	1.37	1.32
2	D	401	NAI	C6A-N6A	3.38	1.46	1.34
2	C	401	NAI	C6N-N1N	3.24	1.45	1.37
2	B	401	NAI	C5B-C4B	3.16	1.61	1.51
2	D	401	NAI	C2A-N3A	3.16	1.37	1.32
2	B	401	NAI	O2D-C2D	3.08	1.50	1.43
2	A	401	NAI	C7N-C3N	3.07	1.55	1.48
2	D	401	NAI	C7N-C3N	3.03	1.55	1.48
2	C	401	NAI	C6A-N6A	3.02	1.45	1.34
2	A	401	NAI	C6N-N1N	3.00	1.44	1.37
2	B	401	NAI	C7N-C3N	2.99	1.55	1.48
2	D	401	NAI	C5D-C4D	2.97	1.60	1.51
2	B	401	NAI	C5D-C4D	2.95	1.60	1.51
2	A	401	NAI	C5D-C4D	2.91	1.60	1.51
2	D	401	NAI	C6N-N1N	2.89	1.44	1.37
2	D	401	NAI	C5A-C4A	-2.74	1.33	1.40
2	C	401	NAI	C5D-C4D	2.72	1.60	1.51
2	A	401	NAI	C5A-C4A	-2.68	1.33	1.40
2	C	401	NAI	C7N-C3N	2.61	1.54	1.48
2	A	401	NAI	C5B-C4B	2.51	1.59	1.51
2	D	401	NAI	C5B-C4B	2.49	1.59	1.51
2	A	401	NAI	O3D-C3D	-2.49	1.37	1.43
2	B	401	NAI	O3D-C3D	-2.46	1.37	1.43
2	D	401	NAI	O3D-C3D	-2.42	1.37	1.43
2	C	401	NAI	C5A-C4A	-2.41	1.34	1.40
2	C	401	NAI	C5B-C4B	2.39	1.59	1.51
2	D	401	NAI	O3B-C3B	-2.34	1.37	1.43
2	B	401	NAI	C4N-C5N	2.32	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C4N-C5N	2.28	1.54	1.48
2	C	401	NAI	O2D-C2D	2.26	1.48	1.43
2	A	401	NAI	PN-O5D	2.24	1.68	1.59
2	D	401	NAI	PN-O5D	2.09	1.67	1.59
2	B	401	NAI	C5A-C4A	-2.07	1.35	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAI	C5A-C6A-N6A	7.48	131.72	120.35
2	A	401	NAI	C5A-C6A-N6A	6.61	130.39	120.35
2	D	401	NAI	N3A-C2A-N1A	-6.59	118.38	128.68
2	B	401	NAI	C5A-C6A-N6A	6.57	130.34	120.35
2	B	401	NAI	O4B-C1B-C2B	-5.93	98.26	106.93
2	A	401	NAI	N3A-C2A-N1A	-5.75	119.69	128.68
2	D	401	NAI	N6A-C6A-N1A	-5.45	107.27	118.57
2	C	401	NAI	N3A-C2A-N1A	-5.14	120.65	128.68
2	B	401	NAI	N3A-C2A-N1A	-4.88	121.05	128.68
2	C	401	NAI	O4B-C1B-C2B	-4.63	100.16	106.93
2	C	401	NAI	C5A-C6A-N6A	4.61	127.35	120.35
2	D	401	NAI	C3N-C2N-N1N	-4.52	116.65	123.10
2	B	401	NAI	N6A-C6A-N1A	-4.41	109.42	118.57
2	A	401	NAI	N6A-C6A-N1A	-4.39	109.46	118.57
4	D	402	OAA	O3-C3-C2	3.61	126.45	120.75
2	A	401	NAI	C1D-N1N-C2N	-3.49	115.30	121.11
2	D	401	NAI	C1B-N9A-C4A	-3.38	120.70	126.64
2	C	401	NAI	N6A-C6A-N1A	-3.32	111.69	118.57
2	B	401	NAI	C3B-C2B-C1B	3.27	105.89	100.98
2	D	401	NAI	C1D-N1N-C2N	-3.22	115.76	121.11
2	A	401	NAI	O4B-C1B-C2B	-3.10	102.39	106.93
2	A	401	NAI	C4D-O4D-C1D	-3.05	102.75	109.47
2	B	401	NAI	C1D-N1N-C2N	-3.01	116.11	121.11
2	A	401	NAI	C1B-N9A-C4A	-2.96	121.44	126.64
4	C	402	OAA	C1-C2-C3	-2.81	110.49	115.51
2	C	401	NAI	C2B-C3B-C4B	-2.72	97.35	102.64
2	B	401	NAI	C4D-O4D-C1D	-2.67	103.58	109.47
2	C	401	NAI	O4B-C4B-C3B	2.64	110.34	105.11
2	B	401	NAI	C2B-C3B-C4B	-2.55	97.69	102.64
2	A	401	NAI	C5D-C4D-C3D	-2.54	105.66	115.18
2	C	401	NAI	C3B-C2B-C1B	2.42	104.62	100.98
2	D	401	NAI	PN-O3-PA	-2.34	124.80	132.83
2	C	401	NAI	C4D-O4D-C1D	-2.33	104.33	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAI	C5B-C4B-C3B	-2.33	106.44	115.18
2	D	401	NAI	O4B-C4B-C3B	2.33	109.72	105.11
2	C	401	NAI	O3B-C3B-C4B	2.32	117.77	111.05
2	D	401	NAI	O5B-C5B-C4B	-2.30	101.08	108.99
2	C	401	NAI	C3N-C2N-N1N	-2.26	119.87	123.10
2	A	401	NAI	PN-O3-PA	-2.26	125.07	132.83
2	C	401	NAI	O4B-C4B-C5B	-2.23	102.05	109.37
2	B	401	NAI	C1B-N9A-C4A	-2.21	122.76	126.64
2	C	401	NAI	C1D-N1N-C2N	-2.19	117.47	121.11
2	C	401	NAI	O3D-C3D-C2D	-2.17	104.80	111.82
2	D	401	NAI	C4D-O4D-C1D	-2.16	104.71	109.47
2	A	401	NAI	O5B-C5B-C4B	-2.09	101.78	108.99
2	B	401	NAI	C3N-C2N-N1N	-2.08	120.13	123.10
2	B	401	NAI	PN-O3-PA	-2.07	125.72	132.83
2	A	401	NAI	C5B-C4B-C3B	-2.01	107.63	115.18

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C2N
2	B	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	C1-C2-C3-O3
4	C	402	OAA	C1-C2-C3-C4
2	D	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-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	C	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	C5B-O5B-PA-O1A

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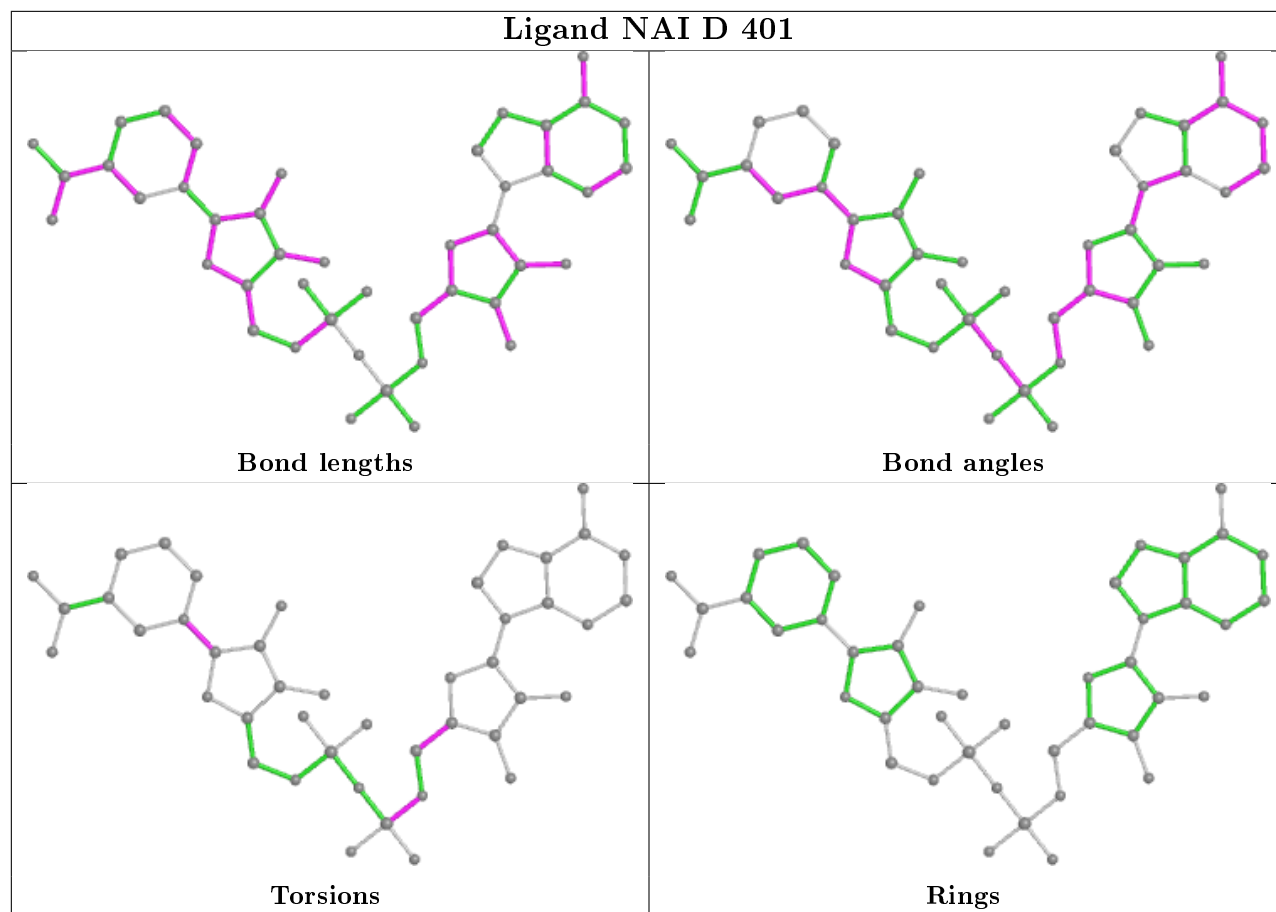| Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C2N-C3N-C7N-N7N
2	D	401	NAI	O4B-C4B-C5B-O5B

There are no ring outliers.
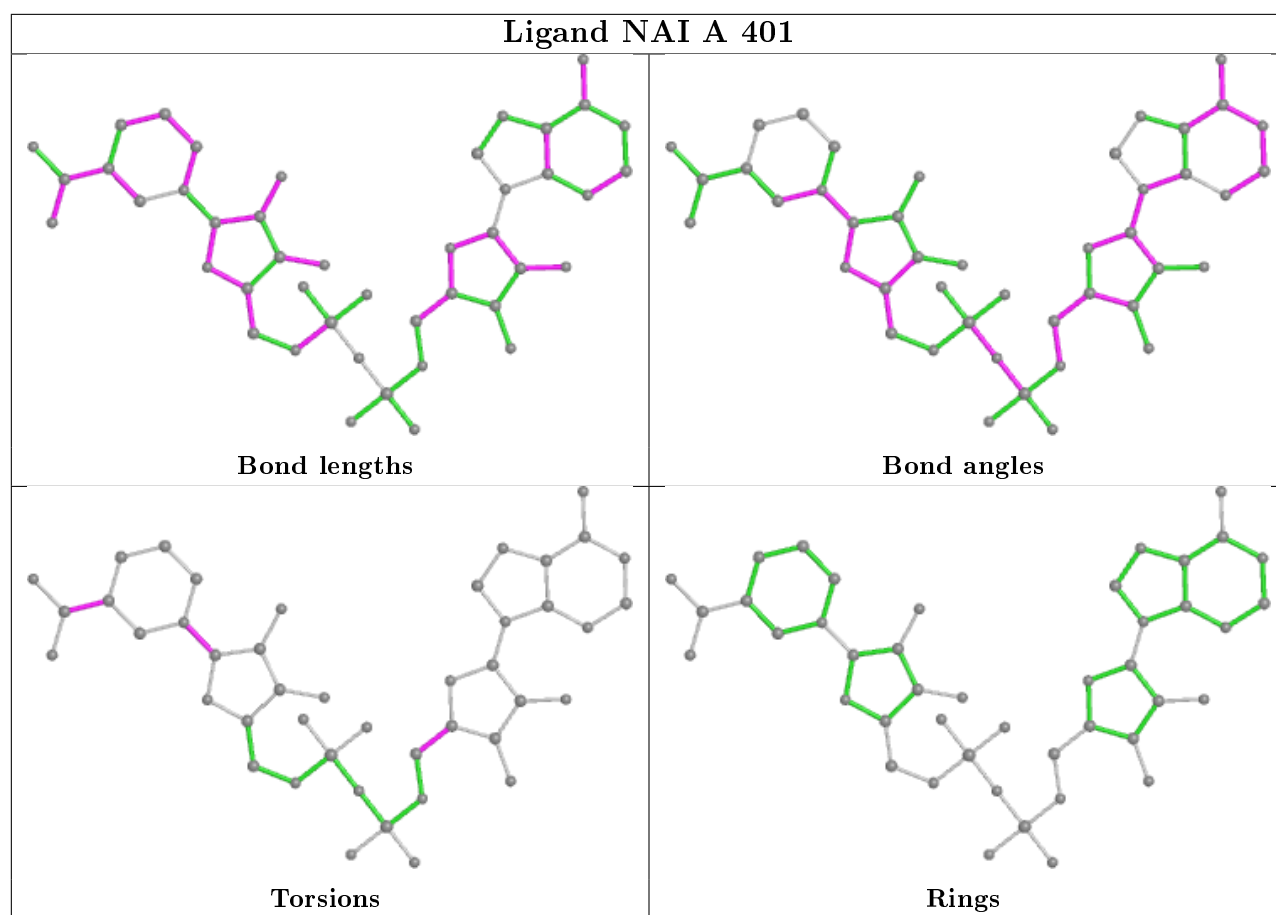
3 monomers are involved in 4 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI A 401

Bond lengths

Bond angles

Torsions

Rings
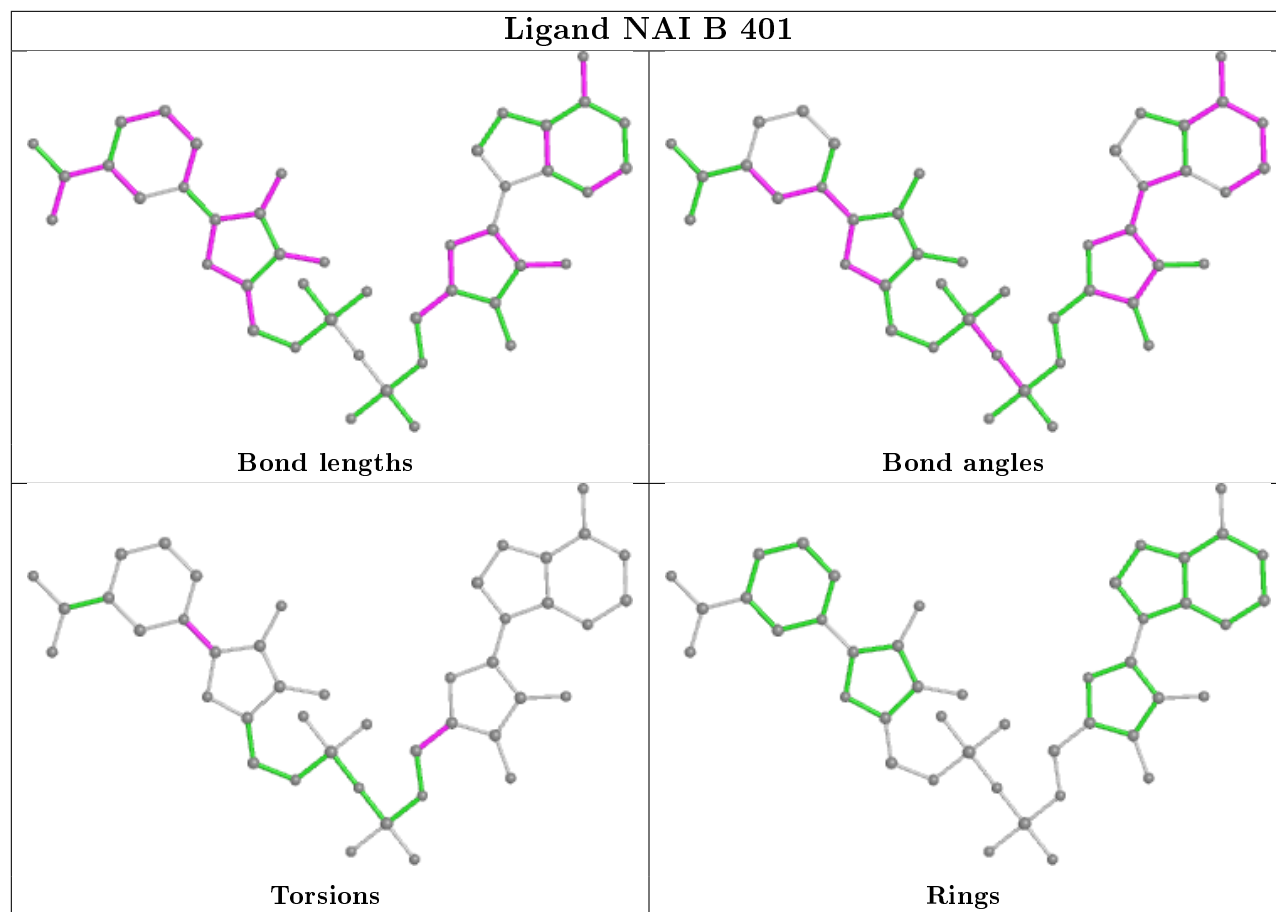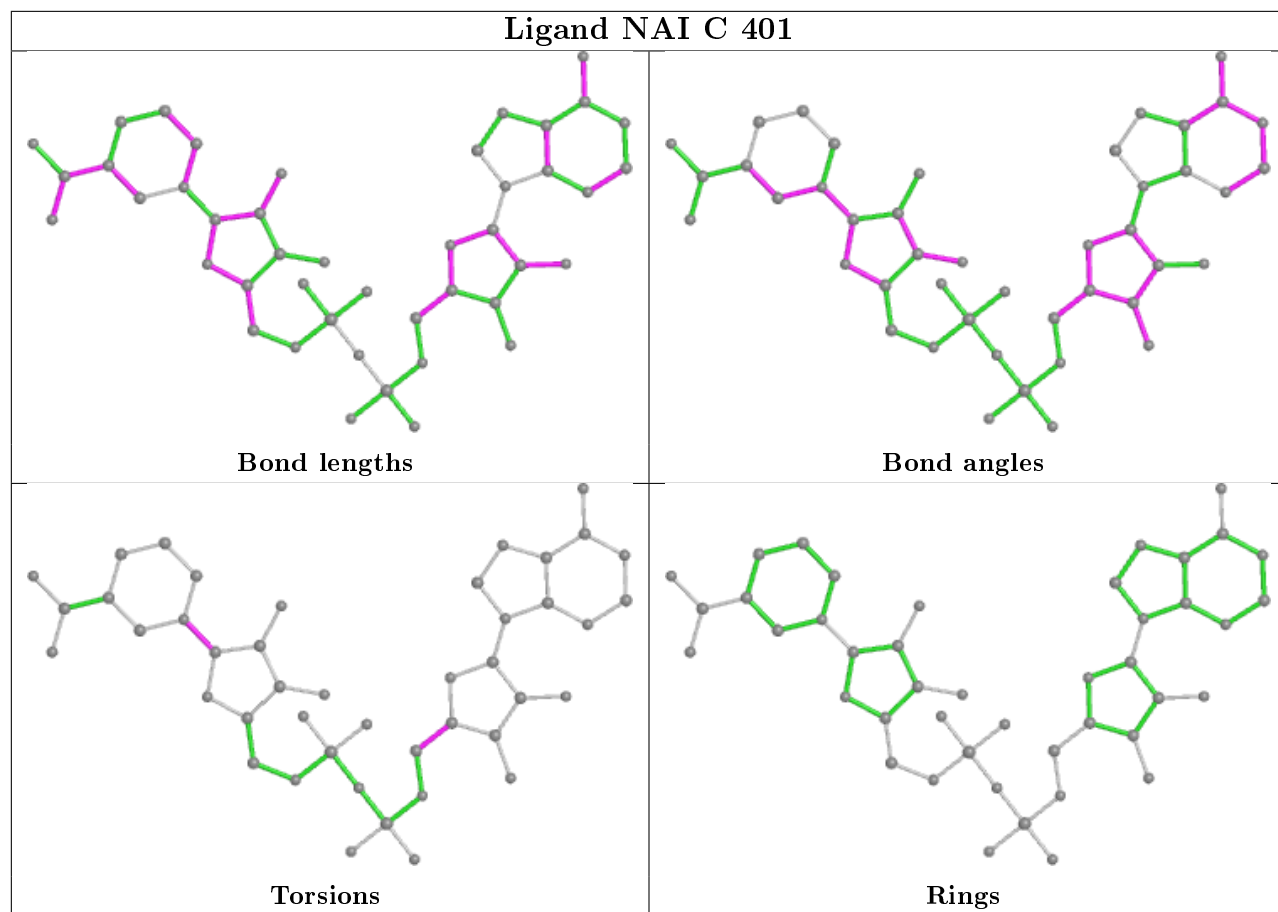
5.7 Other polymers (i)

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	331/332 (99%)	0.20	25 (7%)	13	15	16, 29, 72, 117	0
1	B	331/332 (99%)	0.09	20 (6%)	21	23	17, 28, 55, 95	0
1	C	331/332 (99%)	-0.04	15 (4%)	33	34	16, 27, 53, 88	0
1	D	331/332 (99%)	0.14	20 (6%)	21	23	17, 27, 64, 107	0
All	All	1324/1328 (99%)	0.10	80 (6%)	21	23	16, 28, 60, 117	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	GLN	11.0
1	A	15	GLU	8.6
1	D	331	PHE	8.4
1	A	102	GLY	6.1
1	A	103	GLU	6.1
1	C	330	GLN	5.9
1	B	100	GLN	5.8
1	D	98	ARG	5.8
1	D	101	GLU	5.7
1	A	13	LYS	5.4
1	A	331	PHE	5.2
1	D	102	GLY	5.0
1	C	14	GLU	4.7
1	B	15	GLU	4.7
1	D	106	LEU	4.6
1	B	331	PHE	4.5
1	C	15	GLU	4.5
1	D	14	GLU	4.4
1	D	103	GLU	4.3
1	C	16	HIS	4.2
1	A	1	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	GLN	4.1
1	D	221	ALA	4.1
1	D	104	SER	4.0
1	B	221	ALA	4.0
1	B	13	LYS	3.9
1	A	107	ASN	3.8
1	A	99	GLN	3.7
1	D	105	ARG	3.6
1	A	101	GLU	3.6
1	D	238	TYR	3.6
1	A	100	GLN	3.6
1	D	330	GLN	3.6
1	A	108	LEU	3.6
1	C	220	ASP	3.5
1	D	223	LYS	3.5
1	B	327	LYS	3.4
1	A	106	LEU	3.4
1	A	223	LYS	3.3
1	A	104	SER	3.2
1	B	1	ALA	3.2
1	A	14	GLU	3.2
1	B	101	GLU	3.1
1	A	238	TYR	3.0
1	C	221	ALA	3.0
1	A	276	LEU	2.9
1	B	16	HIS	2.9
1	A	105	ARG	2.9
1	A	16	HIS	2.9
1	A	221	ALA	2.9
1	D	108	LEU	2.8
1	D	15	GLU	2.8
1	A	328	GLU	2.8
1	B	104	SER	2.7
1	A	98	ARG	2.7
1	B	3	LEU	2.7
1	C	320	ASP	2.7
1	B	107	ASN	2.6
1	B	324	GLY	2.6
1	B	14	GLU	2.5
1	B	103	GLU	2.5
1	C	327	LYS	2.4
1	C	17	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	97	ALA	2.4
1	B	317	LYS	2.3
1	C	1	ALA	2.3
1	B	159	GLY	2.3
1	C	283	LYS	2.3
1	C	118	PHE	2.3
1	D	16	HIS	2.3
1	A	220	ASP	2.2
1	D	107	ASN	2.2
1	C	317	LYS	2.1
1	A	329	LEU	2.1
1	B	283	LYS	2.1
1	B	99	GLN	2.1
1	C	223	LYS	2.0
1	A	134	VAL	2.0
1	B	225	GLN	2.0
1	C	316	LYS	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 carbohydrates 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
4	OAA	D	402	9/9	0.74	0.24	32,42,52,56	11
4	OAA	C	402	9/9	0.82	0.32	24,29,34,36	11
2	NAI	D	401	44/44	0.94	0.11	26,40,50,58	0
3	SO4	A	402	5/5	0.95	0.10	31,36,37,42	0
2	NAI	A	401	44/44	0.95	0.09	25,37,54,58	0
3	SO4	B	402	5/5	0.95	0.10	34,38,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	SO4	D	403	5/5	0.97	0.10	28,29,41,44	0
2	NAI	C	401	44/44	0.97	0.09	19,26,35,42	0
3	SO4	C	403	5/5	0.98	0.06	32,34,42,44	0
2	NAI	B	401	44/44	0.98	0.11	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.
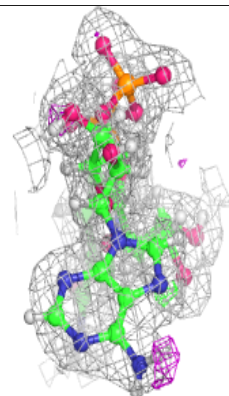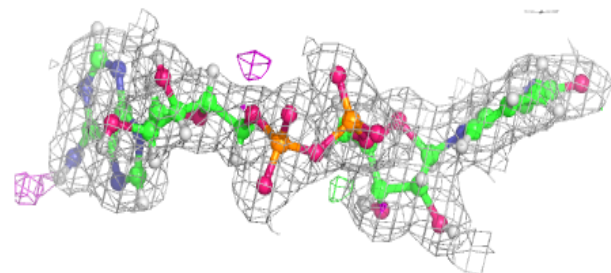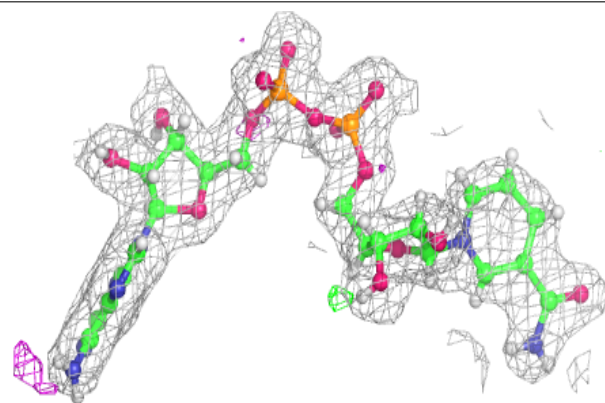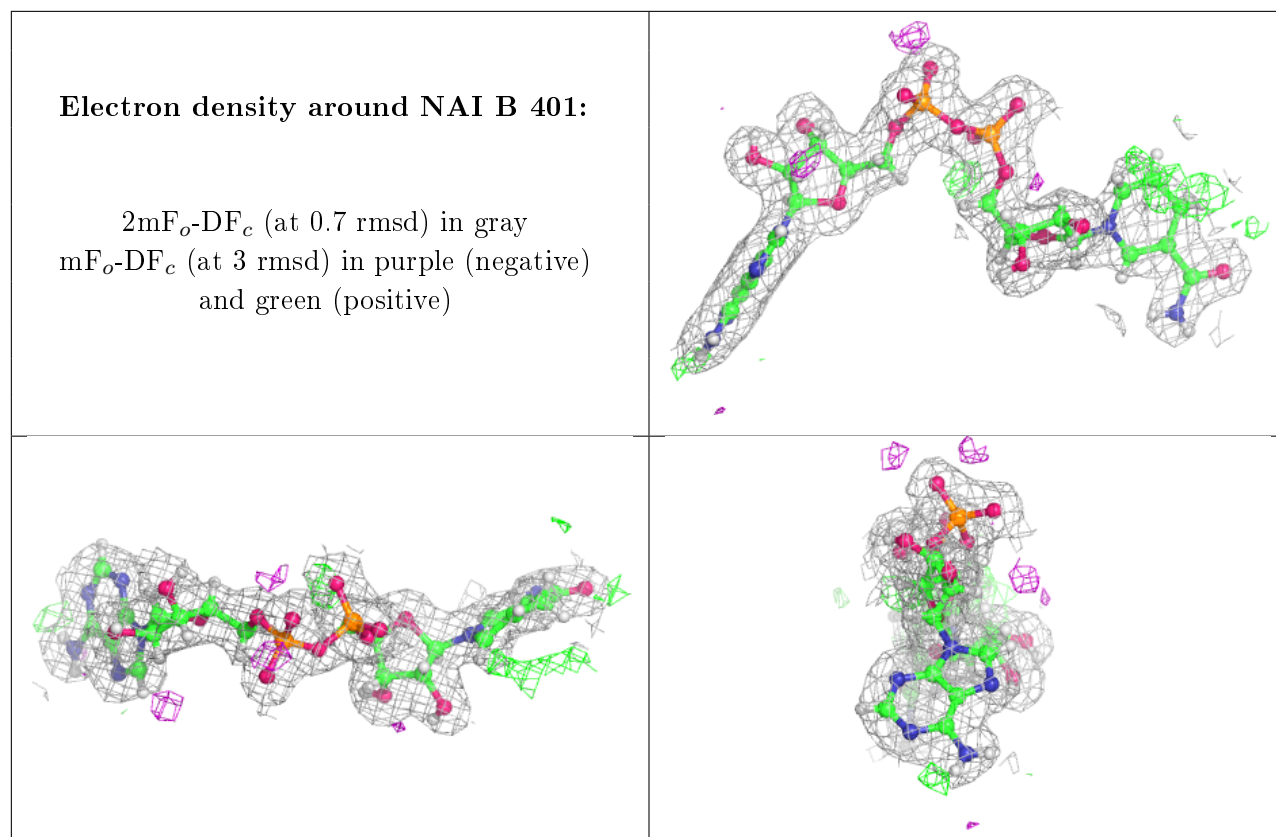

Electron density around NAI D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
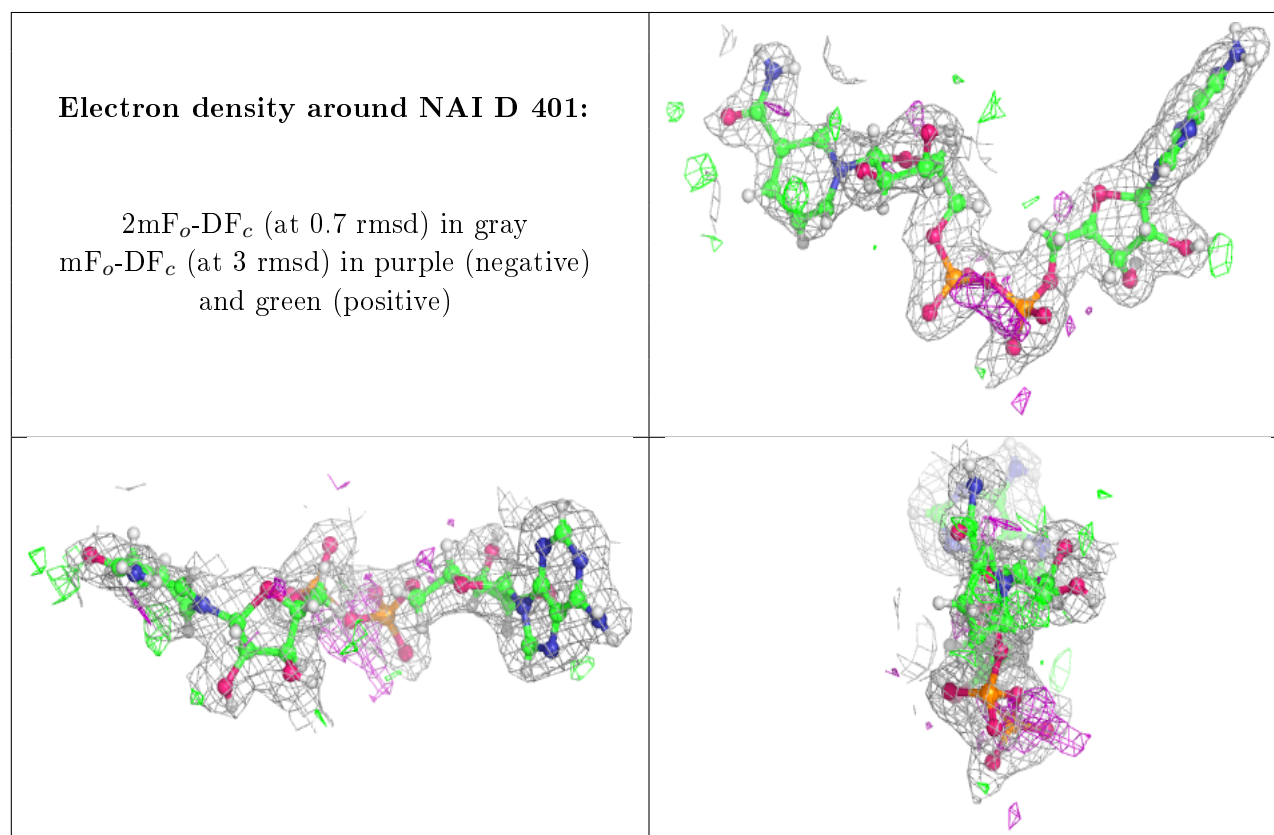
Electron density around NAI A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
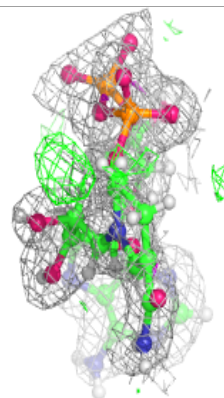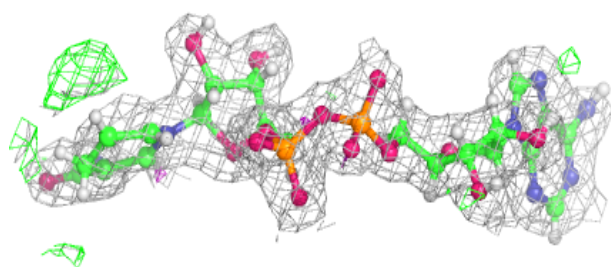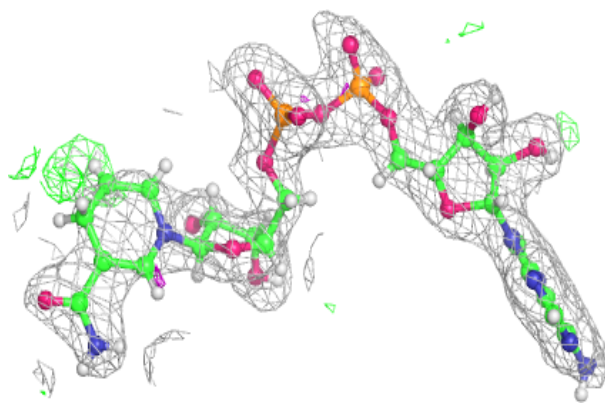
Electron density around NAI C 401:

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

Electron density around 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 ⓘ

There are no such residues in this entry.