Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:48 PM UTC

PDB ID	:	5YAP / pdb_00005yap
Title	:	Crystal structure of scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity complexed with L-glucono-1,5-lactone
Authors	:	Fukano, K.; Shimizu, T.; Sasaki, Y.; Nakamura, A.; Yajima, S.
Deposited on	:	2017-09-01
Resolution	:	1.80 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:

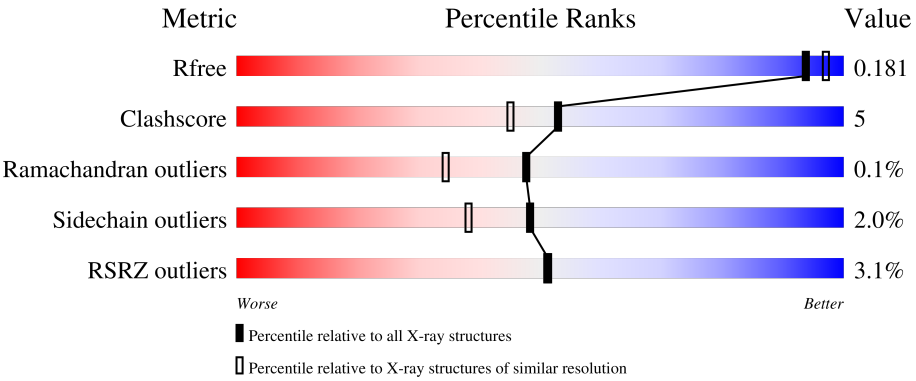
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	380	2% 87% 8%
1	B	380	4% 86% 10%
1	C	380	4% 87% 9%
1	D	380	2% 88% 7% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12183 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 Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2785	1744	510	513	18			
1	B	367	Total	C	N	O	S	0	0	0
			2793	1750	511	514	18			
1	C	366	Total	C	N	O	S	0	0	0
			2785	1744	510	513	18			
1	D	362	Total	C	N	O	S	0	0	0
			2755	1724	506	507	18			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	SER	ASN	engineered mutation	UNP K7ZP76
A	373	LEU	-	expression tag	UNP K7ZP76
A	374	GLU	-	expression tag	UNP K7ZP76
A	375	HIS	-	expression tag	UNP K7ZP76
A	376	HIS	-	expression tag	UNP K7ZP76
A	377	HIS	-	expression tag	UNP K7ZP76
A	378	HIS	-	expression tag	UNP K7ZP76
A	379	HIS	-	expression tag	UNP K7ZP76
A	380	HIS	-	expression tag	UNP K7ZP76
B	72	SER	ASN	engineered mutation	UNP K7ZP76
B	373	LEU	-	expression tag	UNP K7ZP76
B	374	GLU	-	expression tag	UNP K7ZP76
B	375	HIS	-	expression tag	UNP K7ZP76
B	376	HIS	-	expression tag	UNP K7ZP76
B	377	HIS	-	expression tag	UNP K7ZP76
B	378	HIS	-	expression tag	UNP K7ZP76
B	379	HIS	-	expression tag	UNP K7ZP76
B	380	HIS	-	expression tag	UNP K7ZP76
C	72	SER	ASN	engineered mutation	UNP K7ZP76
C	373	LEU	-	expression tag	UNP K7ZP76

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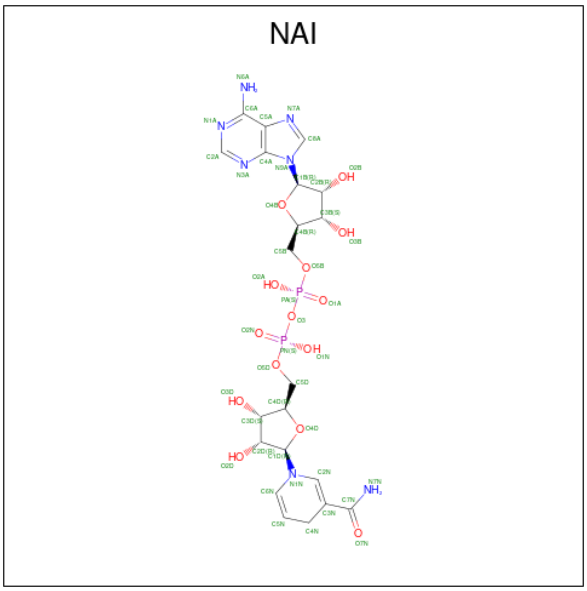
Chain	Residue	Modelled	Actual	Comment	Reference
C	374	GLU	-	expression tag	UNP K7ZP76
C	375	HIS	-	expression tag	UNP K7ZP76
C	376	HIS	-	expression tag	UNP K7ZP76
C	377	HIS	-	expression tag	UNP K7ZP76
C	378	HIS	-	expression tag	UNP K7ZP76
C	379	HIS	-	expression tag	UNP K7ZP76
C	380	HIS	-	expression tag	UNP K7ZP76
D	72	SER	ASN	engineered mutation	UNP K7ZP76
D	373	LEU	-	expression tag	UNP K7ZP76
D	374	GLU	-	expression tag	UNP K7ZP76
D	375	HIS	-	expression tag	UNP K7ZP76
D	376	HIS	-	expression tag	UNP K7ZP76
D	377	HIS	-	expression tag	UNP K7ZP76
D	378	HIS	-	expression tag	UNP K7ZP76
D	379	HIS	-	expression tag	UNP K7ZP76
D	380	HIS	-	expression tag	UNP K7ZP76

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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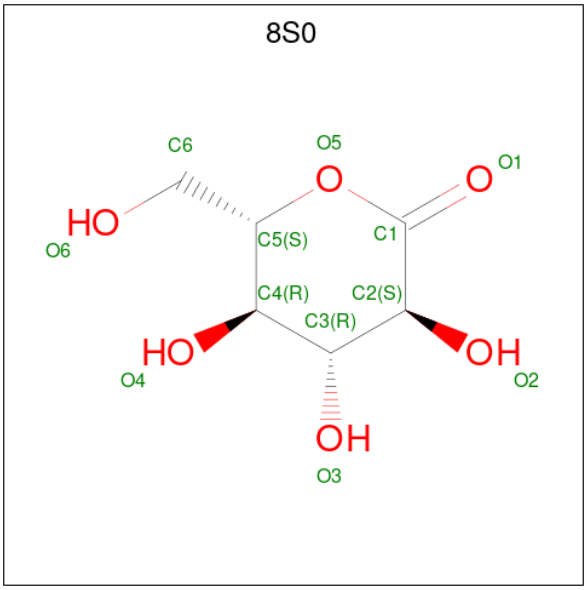
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is L-glucono-1,5-lactone (CCD ID: 8S0) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

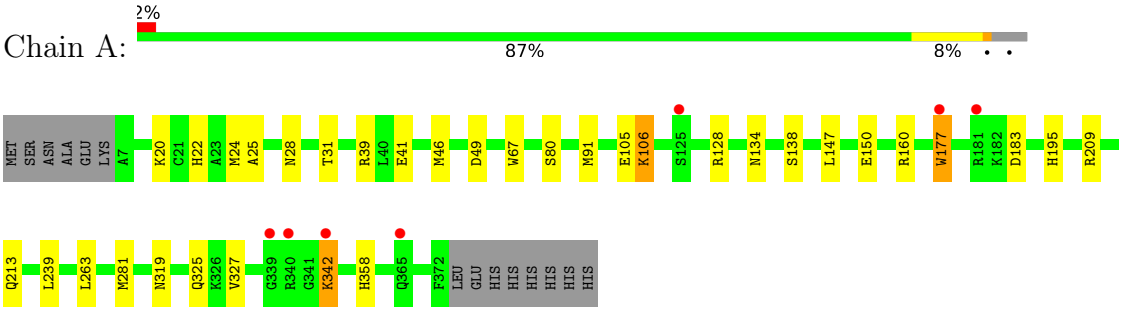
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	202	Total	O	0	0
			202	202		
4	C	188	Total	O	0	0
			188	188		
4	D	236	Total	O	0	0
			236	236		

3 Residue-property plots (i)

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

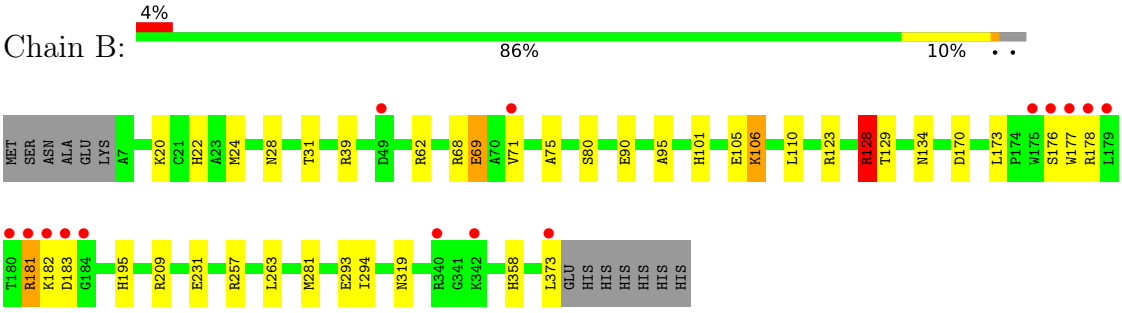
• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain A:



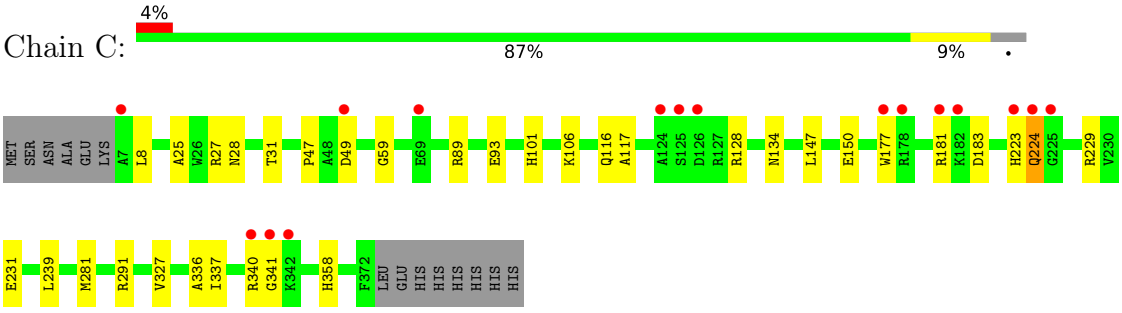
• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain B:



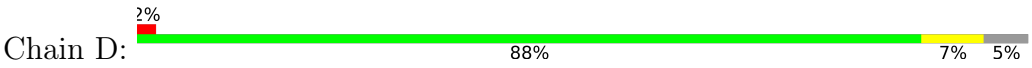
• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

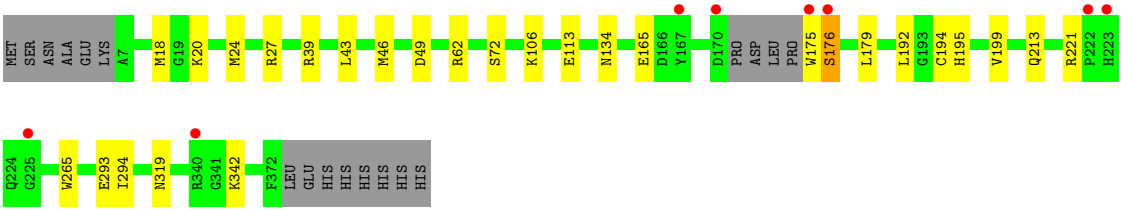
Chain C:



• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain D:




MET SER ASN ALA GLU LYS A7 M18 G19 K20 M24 R27 R39 L43 M46 D49 R62 S72 K106 E113 N134 E165 D166 Y167 D170 PRO ASP LEU PRO W175 S176 L179 L192 G193 C194 H195 V199 Q213 R221 P222 H223
Q224 G225 W265 E293 I294 N319 R340 G341 K342 F372 LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.57Å 121.18Å 140.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 1.80 31.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.50-1.80) 99.6 (31.50-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.163 , 0.170 0.173 , 0.181	Depositor DCC
R_{free} test set	6848 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12183	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, 8S0

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	0.69	0/2851	0.84	0/3865
1	B	0.72	1/2859 (0.0%)	0.88	3/3876 (0.1%)
1	C	0.68	0/2851	0.84	0/3865
1	D	0.68	0/2818	0.84	1/3816 (0.0%)
All	All	0.69	1/11379 (0.0%)	0.85	4/15422 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	THR	C-O	-6.51	1.15	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	ARG	NE-CZ-NH2	-8.75	111.33	119.20
1	B	128	ARG	CG-CD-NE	-7.42	95.68	112.00
1	B	128	ARG	CD-NE-CZ	5.87	132.62	124.40
1	D	62	ARG	CG-CD-NE	5.31	123.68	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2785	0	2702	28	0
1	B	2793	0	2713	36	0
1	C	2785	0	2702	29	0
1	D	2755	0	2672	29	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	1	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
3	C	12	0	0	0	0
4	A	227	0	0	9	0
4	B	202	0	0	11	0
4	C	188	0	0	15	0
4	D	236	0	0	13	0
All	All	12183	0	10897	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (110) 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:C:49:ASP:HB2	4:C:663:HOH:O	1.50	1.09
1:D:176:SER:HB3	4:D:707:HOH:O	1.55	1.07
1:B:294:ILE:HG13	4:B:503:HOH:O	1.55	1.05
1:A:49:ASP:HB2	4:A:711:HOH:O	1.57	1.03
1:C:89:ARG:NH1	1:C:93:GLU:OE2	1.94	1.01
1:A:39:ARG:NH1	1:A:41:GLU:OE2	1.96	0.97
1:D:342:LYS:HE3	4:D:816:HOH:O	1.68	0.90
1:D:49:ASP:HB2	4:D:814:HOH:O	1.74	0.88
1:D:294:ILE:HG13	4:D:698:HOH:O	1.77	0.84
1:B:183:ASP:HA	4:B:504:HOH:O	1.78	0.81
4:C:503:HOH:O	1:D:24:MET:CE	2.28	0.81
1:A:209:ARG:HD2	4:C:671:HOH:O	1.81	0.79
1:A:342:LYS:HD3	4:A:718:HOH:O	1.83	0.78
4:A:505:HOH:O	1:B:24:MET:HE2	1.84	0.77
1:B:101:HIS:HD2	1:B:128:ARG:H	1.31	0.76
4:C:503:HOH:O	1:D:24:MET:HE2	1.84	0.76
1:A:106:LYS:HE3	1:A:106:LYS:C	2.11	0.75
1:B:373:LEU:HD11	4:B:651:HOH:O	1.89	0.73
1:A:150:GLU:HB2	4:D:601:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:MET:HE2	4:B:654:HOH:O	1.88	0.72
1:C:101:HIS:HD2	1:C:128:ARG:H	1.39	0.70
1:C:116:GLN:CD	4:C:505:HOH:O	2.34	0.69
1:B:181:ARG:HD3	4:B:641:HOH:O	1.90	0.69
1:B:106:LYS:HD3	1:B:195:HIS:NE2	2.08	0.69
1:D:342:LYS:HE2	4:D:605:HOH:O	1.91	0.69
1:B:181:ARG:HD3	1:B:231:GLU:OE1	1.93	0.68
1:D:113:GLU:HG3	4:D:758:HOH:O	1.92	0.68
1:A:106:LYS:HD3	1:A:195:HIS:NE2	2.09	0.67
4:A:505:HOH:O	1:B:24:MET:CE	2.41	0.67
1:A:24:MET:CE	4:B:654:HOH:O	2.42	0.66
1:B:170:ASP:HB3	4:B:663:HOH:O	1.97	0.64
1:B:71:VAL:HG13	1:B:95:ALA:HA	1.82	0.62
1:B:106:LYS:HE3	1:B:106:LYS:C	2.25	0.61
1:D:106:LYS:HD2	1:D:106:LYS:C	2.25	0.61
1:A:319:ASN:HD22	1:B:281:MET:HG2	1.66	0.61
1:D:106:LYS:HD3	1:D:194:CYS:SG	2.42	0.59
1:A:177:TRP:HD1	1:A:183:ASP:HB2	1.68	0.59
1:C:340:ARG:HD3	4:C:669:HOH:O	2.02	0.58
1:B:71:VAL:CG1	1:B:95:ALA:HA	2.34	0.58
1:C:223:HIS:CE1	1:C:224:GLN:OE1	2.56	0.57
1:A:281:MET:HG2	1:B:319:ASN:HD22	1.69	0.57
1:B:181:ARG:HG2	1:B:182:LYS:N	2.19	0.57
1:B:170:ASP:OD1	1:B:257:ARG:NH1	2.36	0.57
1:B:294:ILE:C	4:B:503:HOH:O	2.47	0.56
1:C:281:MET:HG2	1:D:319:ASN:HD22	1.70	0.56
1:D:46:MET:HE3	4:D:811:HOH:O	2.05	0.56
1:B:176:SER:OG	1:B:178:ARG:HB2	2.06	0.55
1:B:22:HIS:HE1	1:B:105:GLU:OE2	1.89	0.54
1:A:22:HIS:HE1	1:A:105:GLU:OE2	1.91	0.53
1:B:293:GLU:HG2	1:C:147:LEU:HD21	1.90	0.53
1:C:89:ARG:NH1	1:C:117:ALA:HB1	2.24	0.53
1:D:39:ARG:NH2	4:D:603:HOH:O	2.42	0.52
1:A:22:HIS:HD2	1:A:80:SER:OG	1.92	0.52
1:B:177:TRP:CD1	1:B:177:TRP:H	2.26	0.52
1:A:31:THR:O	1:B:20:LYS:HE3	2.10	0.52
1:A:342:LYS:HD2	4:A:696:HOH:O	2.09	0.51
1:A:106:LYS:HE3	1:A:106:LYS:O	2.11	0.50
1:B:209:ARG:HH22	1:D:213:GLN:HE21	1.60	0.50
1:D:179:LEU:CD1	1:D:221:ARG:HD2	2.42	0.50
1:D:175:TRP:CE3	1:D:221:ARG:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:CD	1:B:231:GLU:OE1	2.59	0.49
1:B:358:HIS:HE1	4:B:529:HOH:O	1.95	0.49
1:B:373:LEU:H	1:B:373:LEU:HD12	1.78	0.49
1:B:22:HIS:HD2	1:B:80:SER:OG	1.96	0.48
1:C:181:ARG:CZ	4:C:504:HOH:O	2.62	0.48
1:C:89:ARG:NH1	1:C:117:ALA:CB	2.76	0.47
1:C:181:ARG:NH1	4:C:504:HOH:O	2.47	0.47
1:A:150:GLU:CB	4:D:601:HOH:O	2.53	0.47
1:C:47:PRO:HG2	4:C:663:HOH:O	2.14	0.47
1:C:177:TRP:CD1	1:C:177:TRP:H	2.32	0.47
1:A:342:LYS:CD	4:A:696:HOH:O	2.63	0.47
1:B:123:ARG:CZ	4:B:523:HOH:O	2.63	0.46
1:B:68:ARG:NH2	1:B:90:GLU:OE2	2.48	0.46
4:C:503:HOH:O	1:D:24:MET:HE1	2.03	0.46
1:D:106:LYS:HE2	1:D:195:HIS:NE2	2.30	0.46
1:B:62:ARG:NH1	1:B:69:GLU:OE2	2.37	0.46
1:D:18:MET:HE3	2:D:500:NAI:H4N	1.98	0.46
1:C:181:ARG:HG3	4:C:504:HOH:O	2.15	0.45
1:D:27:ARG:NH1	4:D:607:HOH:O	2.49	0.45
1:D:165:GLU:HG2	1:D:192:LEU:HD11	1.97	0.45
1:C:27:ARG:HD3	1:D:27:ARG:HE	1.80	0.45
1:C:116:GLN:NE2	4:C:505:HOH:O	2.47	0.45
1:D:106:LYS:HE2	4:D:771:HOH:O	2.16	0.45
1:C:89:ARG:HH12	1:C:117:ALA:HB1	1.81	0.45
1:A:138:SER:HB3	1:A:325:GLN:HE21	1.82	0.44
1:B:39:ARG:NH2	1:B:75:ALA:O	2.51	0.44
1:B:110:LEU:HD11	4:B:504:HOH:O	2.16	0.44
1:A:147:LEU:HD21	1:D:293:GLU:HG2	1.98	0.44
1:A:20:LYS:HE3	1:B:31:THR:O	2.18	0.43
1:A:239:LEU:HG	1:C:239:LEU:HG	1.99	0.43
1:C:291:ARG:NH2	4:C:501:HOH:O	2.40	0.43
1:A:25:ALA:HA	1:A:327:VAL:HG22	1.99	0.43
1:A:213:GLN:NE2	4:A:503:HOH:O	2.48	0.43
1:C:27:ARG:NH2	4:C:507:HOH:O	2.51	0.43
1:A:67:TRP:CD1	1:A:91:MET:HE2	2.54	0.43
1:C:336:ALA:HA	1:C:341:GLY:O	2.19	0.43
1:A:160:ARG:HD2	4:A:504:HOH:O	2.18	0.43
1:C:27:ARG:HH22	1:C:59:GLY:HA3	1.84	0.42
1:C:25:ALA:HA	1:C:327:VAL:HG22	2.01	0.42
1:D:179:LEU:HD11	1:D:221:ARG:HD2	2.02	0.42
1:A:358:HIS:HE1	4:A:533:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LEU:HD12	1:B:373:LEU:N	2.34	0.42
1:D:43:LEU:C	1:D:43:LEU:HD23	2.44	0.42
1:D:72:SER:HB3	4:D:732:HOH:O	2.20	0.42
1:C:31:THR:O	1:D:20:LYS:HE3	2.20	0.41
1:C:358:HIS:HE1	4:C:515:HOH:O	2.03	0.41
1:C:8:LEU:HD21	1:C:337:ILE:HG21	2.02	0.41
1:B:293:GLU:OE2	1:C:150:GLU:OE1	2.39	0.41
1:D:199:VAL:HG11	1:D:265:TRP:CD1	2.56	0.41
1:C:229:ARG:NH1	1:C:231:GLU:HG2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/380 (96%)	354 (97%)	10 (3%)	0	100	100
1	B	365/380 (96%)	360 (99%)	5 (1%)	0	100	100
1	C	364/380 (96%)	357 (98%)	6 (2%)	1 (0%)	36	25
1	D	358/380 (94%)	351 (98%)	7 (2%)	0	100	100
All	All	1451/1520 (96%)	1422 (98%)	28 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	224	GLN

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	275/288 (96%)	267 (97%)	8 (3%)	37	25
1	B	276/288 (96%)	268 (97%)	8 (3%)	37	25
1	C	275/288 (96%)	271 (98%)	4 (2%)	57	49
1	D	271/288 (94%)	269 (99%)	2 (1%)	76	73
All	All	1097/1152 (95%)	1075 (98%)	22 (2%)	48	38

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	46	MET
1	A	106	LYS
1	A	128	ARG
1	A	134	ASN
1	A	177	TRP
1	A	263	LEU
1	A	342	LYS
1	B	28	ASN
1	B	69	GLU
1	B	106	LYS
1	B	128	ARG
1	B	134	ASN
1	B	173	LEU
1	B	181	ARG
1	B	263	LEU
1	C	28	ASN
1	C	106	LYS
1	C	134	ASN
1	C	183	ASP
1	D	134	ASN
1	D	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS

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Mol	Chain	Res	Type
1	A	28	ASN
1	A	213	GLN
1	A	237	GLN
1	A	319	ASN
1	A	325	GLN
1	A	358	HIS
1	B	22	HIS
1	B	28	ASN
1	B	101	HIS
1	B	116	GLN
1	B	319	ASN
1	B	358	HIS
1	B	371	ASN
1	C	28	ASN
1	C	101	HIS
1	C	318	HIS
1	C	335	GLN
1	C	358	HIS
1	D	28	ASN
1	D	213	GLN
1	D	278	GLN
1	D	319	ASN
1	D	325	GLN
1	D	371	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

7 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	8S0	C	402	-	12,12,12	1.36	1 (8%)	15,17,17	1.15	1 (6%)
3	8S0	A	402	-	12,12,12	1.38	1 (8%)	15,17,17	1.45	1 (6%)
2	NAI	C	401	-	47,48,48	1.65	12 (25%)	64,73,73	1.75	13 (20%)
2	NAI	D	500	-	47,48,48	1.74	9 (19%)	64,73,73	1.68	9 (14%)
3	8S0	B	402	-	12,12,12	1.43	2 (16%)	15,17,17	1.04	0
2	NAI	A	401	-	47,48,48	1.59	10 (21%)	64,73,73	1.79	12 (18%)
2	NAI	B	401	-	47,48,48	1.51	10 (21%)	64,73,73	1.88	12 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8S0	C	402	-	-	0/2/22/22	0/1/1/1
3	8S0	A	402	-	-	0/2/22/22	0/1/1/1
2	NAI	C	401	-	-	3/29/72/72	0/5/5/5
2	NAI	D	500	-	-	2/29/72/72	0/5/5/5
3	8S0	B	402	-	-	0/2/22/22	0/1/1/1
2	NAI	A	401	-	-	1/29/72/72	0/5/5/5
2	NAI	B	401	-	-	2/29/72/72	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAI	C5A-N7A	-4.61	1.30	1.39
2	D	500	NAI	C8A-N9A	-4.01	1.30	1.37
2	C	401	NAI	C4A-N9A	-3.80	1.29	1.37
2	B	401	NAI	C8A-N9A	-3.80	1.31	1.37
2	C	401	NAI	C5A-C4A	3.73	1.45	1.39
2	A	401	NAI	C5A-N7A	-3.63	1.32	1.39
3	A	402	8S0	C2-C1	-3.52	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C8A-N9A	-3.51	1.31	1.37
3	C	402	8S0	C2-C1	-3.38	1.44	1.52
2	B	401	NAI	O7N-C7N	-3.31	1.16	1.24
2	C	401	NAI	C5A-N7A	-3.29	1.33	1.39
2	A	401	NAI	C4A-N9A	-3.25	1.30	1.37
2	D	500	NAI	C4A-N9A	-3.04	1.31	1.37
2	C	401	NAI	C8A-N9A	-3.02	1.32	1.37
2	C	401	NAI	PN-O2N	-2.97	1.40	1.50
2	B	401	NAI	C4A-N9A	-2.94	1.31	1.37
2	D	500	NAI	PA-O2A	-2.93	1.41	1.55
3	B	402	8S0	O5-C5	-2.88	1.42	1.46
2	D	500	NAI	C5A-C4A	2.87	1.44	1.39
2	D	500	NAI	PN-O2N	-2.82	1.41	1.50
3	B	402	8S0	C2-C1	-2.76	1.46	1.52
2	A	401	NAI	C5A-C4A	2.74	1.44	1.39
2	D	500	NAI	O7N-C7N	-2.70	1.18	1.24
2	B	401	NAI	C5A-N7A	-2.66	1.34	1.39
2	D	500	NAI	C6N-N1N	-2.64	1.30	1.37
2	D	500	NAI	PN-O1N	-2.61	1.43	1.55
2	C	401	NAI	O4B-C4B	-2.61	1.39	1.45
2	B	401	NAI	PA-O1A	-2.61	1.41	1.50
2	B	401	NAI	PN-O3	2.56	1.62	1.59
2	C	401	NAI	O7N-C7N	-2.53	1.18	1.24
2	A	401	NAI	PA-O2A	-2.49	1.43	1.55
2	A	401	NAI	PN-O2N	-2.49	1.42	1.50
2	B	401	NAI	C5A-C4A	2.39	1.43	1.39
2	C	401	NAI	C6N-N1N	-2.39	1.31	1.37
2	C	401	NAI	PA-O2A	-2.36	1.44	1.55
2	A	401	NAI	O7N-C7N	-2.35	1.18	1.24
2	C	401	NAI	PN-O3	-2.29	1.57	1.59
2	A	401	NAI	C2A-N1A	-2.23	1.30	1.33
2	B	401	NAI	C4N-C5N	-2.23	1.43	1.49
2	A	401	NAI	PN-O1N	-2.22	1.45	1.55
2	B	401	NAI	C6N-N1N	-2.20	1.31	1.37
2	C	401	NAI	PN-O1N	-2.13	1.45	1.55
2	A	401	NAI	O4B-C4B	-2.11	1.40	1.45
2	B	401	NAI	PA-O2A	-2.11	1.45	1.55
2	C	401	NAI	C5A-C6A	2.07	1.46	1.41

All (48) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	NAI	C5A-C4A-N3A	-6.52	117.74	126.72
2	A	401	NAI	C5A-C4A-N3A	-5.88	118.62	126.72
2	B	401	NAI	N3A-C4A-N9A	5.83	137.08	127.17
2	B	401	NAI	C5A-C4A-N3A	-5.82	118.70	126.72
2	C	401	NAI	C5A-C4A-N3A	-5.75	118.79	126.72
2	D	500	NAI	N3A-C4A-N9A	5.33	136.24	127.17
2	A	401	NAI	N3A-C4A-N9A	5.02	135.70	127.17
2	C	401	NAI	N3A-C4A-N9A	4.99	135.66	127.17
2	A	401	NAI	N3A-C2A-N1A	-4.87	121.21	128.58
2	B	401	NAI	C2A-N3A-C4A	4.41	122.59	111.83
2	A	401	NAI	C2A-N3A-C4A	4.39	122.56	111.83
2	B	401	NAI	N3A-C2A-N1A	-4.20	122.23	128.58
2	C	401	NAI	C2A-N3A-C4A	4.12	121.90	111.83
3	A	402	8S0	O5-C5-C6	-4.11	101.93	106.05
2	D	500	NAI	C2A-N3A-C4A	4.00	121.61	111.83
2	B	401	NAI	O2A-PA-O1A	3.97	130.93	112.44
2	B	401	NAI	N6A-C6A-N1A	3.74	126.71	118.38
2	C	401	NAI	C4A-N9A-C8A	3.72	109.64	105.74
2	B	401	NAI	C5A-C6A-N6A	-3.67	114.20	123.29
2	B	401	NAI	C4A-N9A-C8A	3.65	109.57	105.74
2	C	401	NAI	N3A-C2A-N1A	-3.64	123.07	128.58
2	A	401	NAI	C2A-N1A-C6A	3.39	124.30	118.73
2	D	500	NAI	N3A-C2A-N1A	-3.14	123.83	128.58
2	A	401	NAI	C4A-N9A-C8A	3.06	108.96	105.74
2	D	500	NAI	C4A-C5A-N7A	-3.03	107.12	110.58
2	C	401	NAI	C4A-C5A-N7A	-2.88	107.28	110.58
2	A	401	NAI	C2D-C1D-N1N	2.77	120.11	113.31
2	A	401	NAI	C4A-C5A-N7A	-2.73	107.46	110.58
2	B	401	NAI	O4B-C1B-N9A	2.64	113.16	108.09
2	A	401	NAI	C6N-N1N-C2N	2.57	122.07	119.32
2	A	401	NAI	O2A-PA-O1A	2.56	124.36	112.44
2	C	401	NAI	N6A-C6A-N1A	2.47	123.88	118.38
2	D	500	NAI	C1D-N1N-C2N	-2.44	117.11	121.14
2	A	401	NAI	O4B-C1B-C2B	-2.44	101.39	106.62
2	C	401	NAI	O4B-C1B-C2B	-2.43	101.42	106.62
3	C	402	8S0	O5-C5-C6	-2.39	103.65	106.05
2	A	401	NAI	C6A-C5A-N7A	2.27	136.46	132.09
2	C	401	NAI	O2A-PA-O1A	2.24	122.86	112.44
2	C	401	NAI	C6N-N1N-C2N	2.23	121.71	119.32
2	C	401	NAI	C6A-C5A-N7A	2.21	136.34	132.09
2	C	401	NAI	C5A-C6A-N6A	-2.20	117.83	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	NAI	N6A-C6A-N1A	2.17	123.21	118.38
2	B	401	NAI	O7N-C7N-C3N	-2.17	116.81	120.90
2	D	500	NAI	O4B-C1B-C2B	-2.17	101.98	106.62
2	B	401	NAI	O1N-PN-O2N	2.14	122.40	112.44
2	D	500	NAI	C5A-N7A-C8A	2.12	106.78	103.45
2	B	401	NAI	C5B-C4B-C3B	-2.12	107.58	115.21
2	C	401	NAI	O5D-PN-O2N	-2.03	100.89	108.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	O4D-C1D-N1N-C2N
2	C	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	D	500	NAI	O4D-C1D-N1N-C2N
2	D	500	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	PN-O3-PA-O1A
2	C	401	NAI	PN-O3-PA-O2A

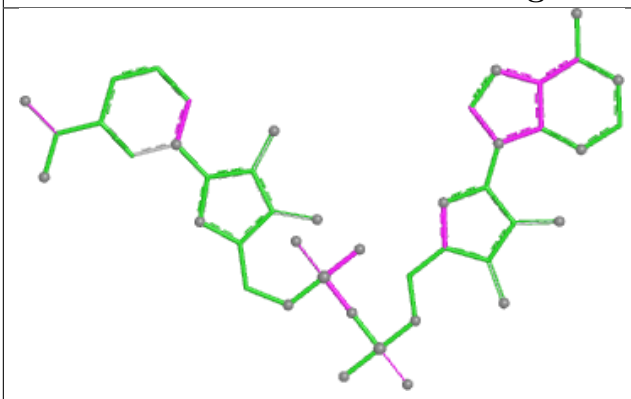
There are no ring outliers.

1 monomer is involved in 1 short contact:

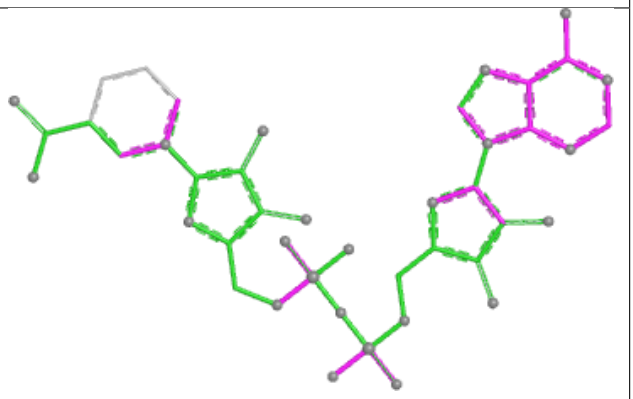
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	NAI	1	0

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.

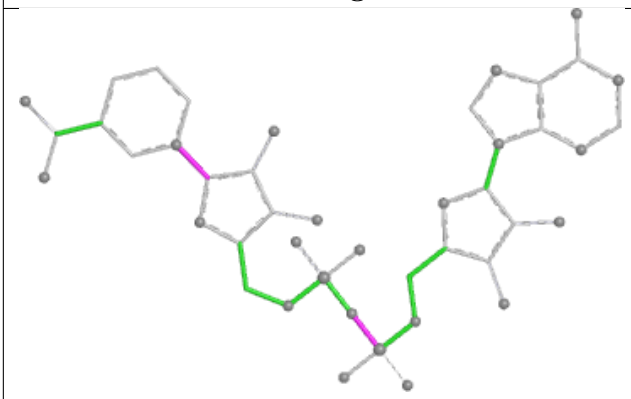
Ligand NAI C 401



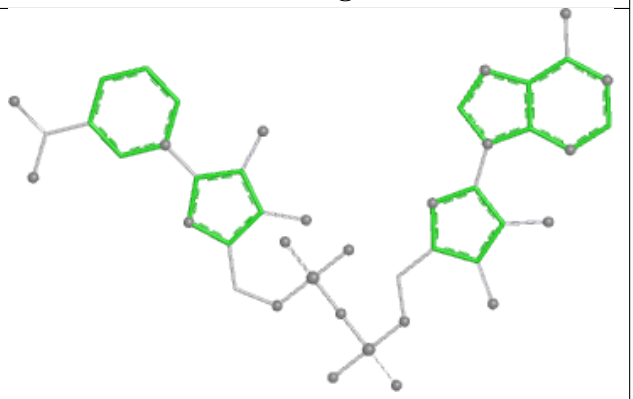
Bond lengths



Bond angles

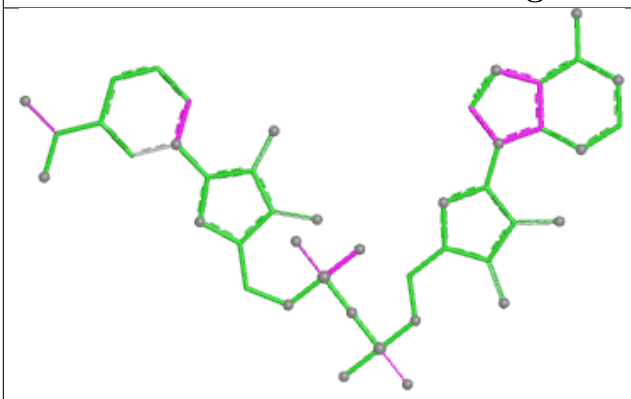


Torsions



Rings

Ligand NAI D 500



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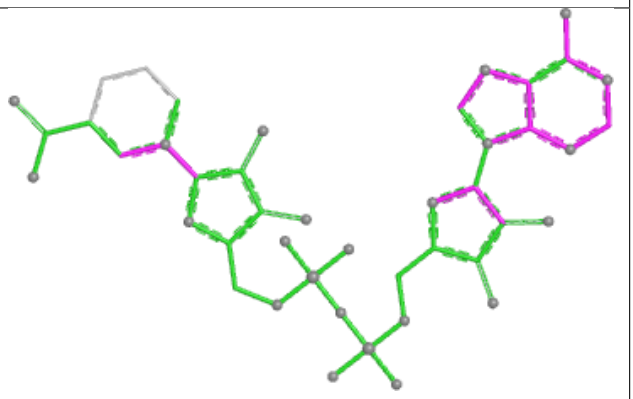
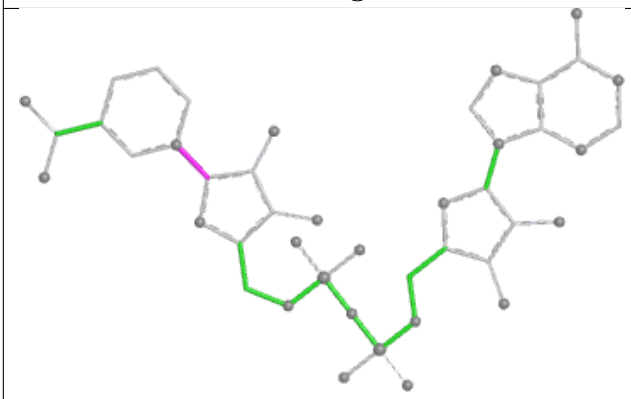


Bond angles



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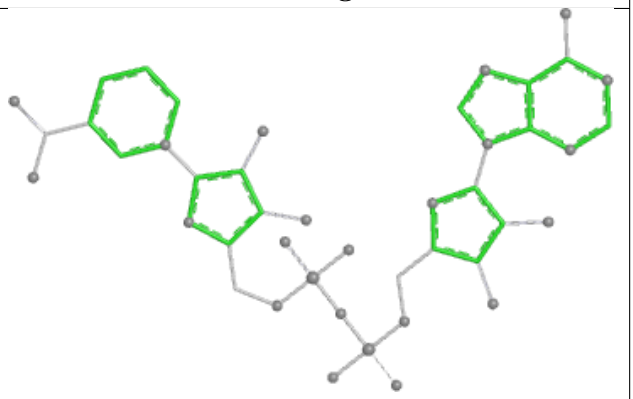
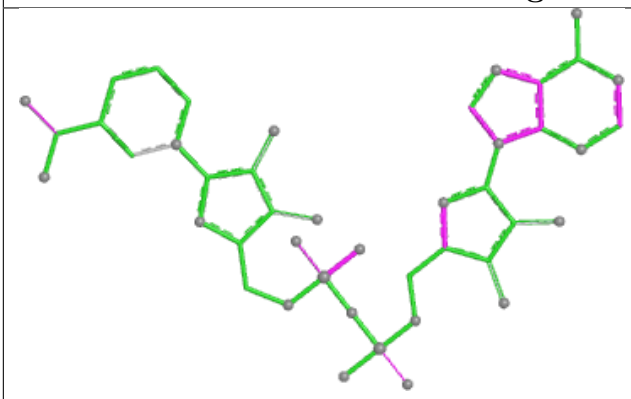
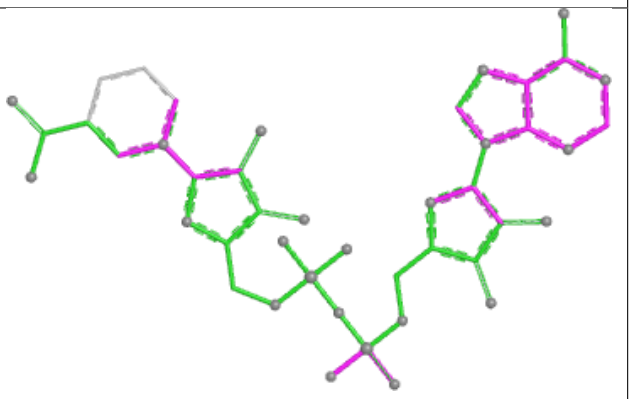


Rings

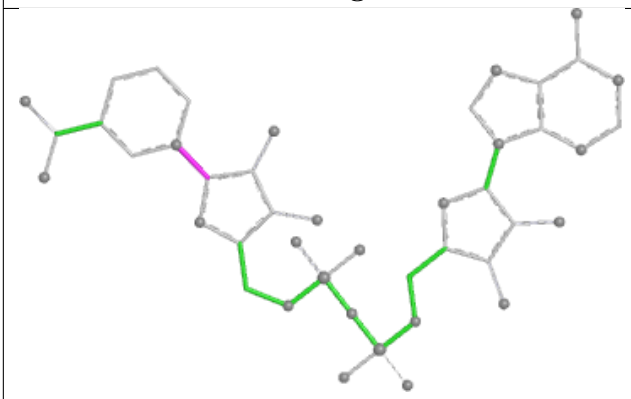
Ligand NAI A 401



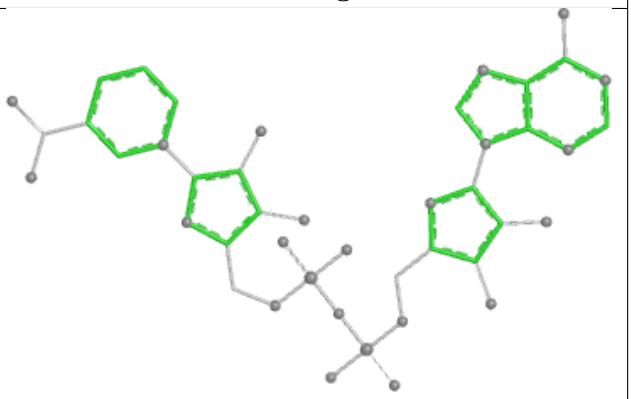
Bond lengths



Bond angles

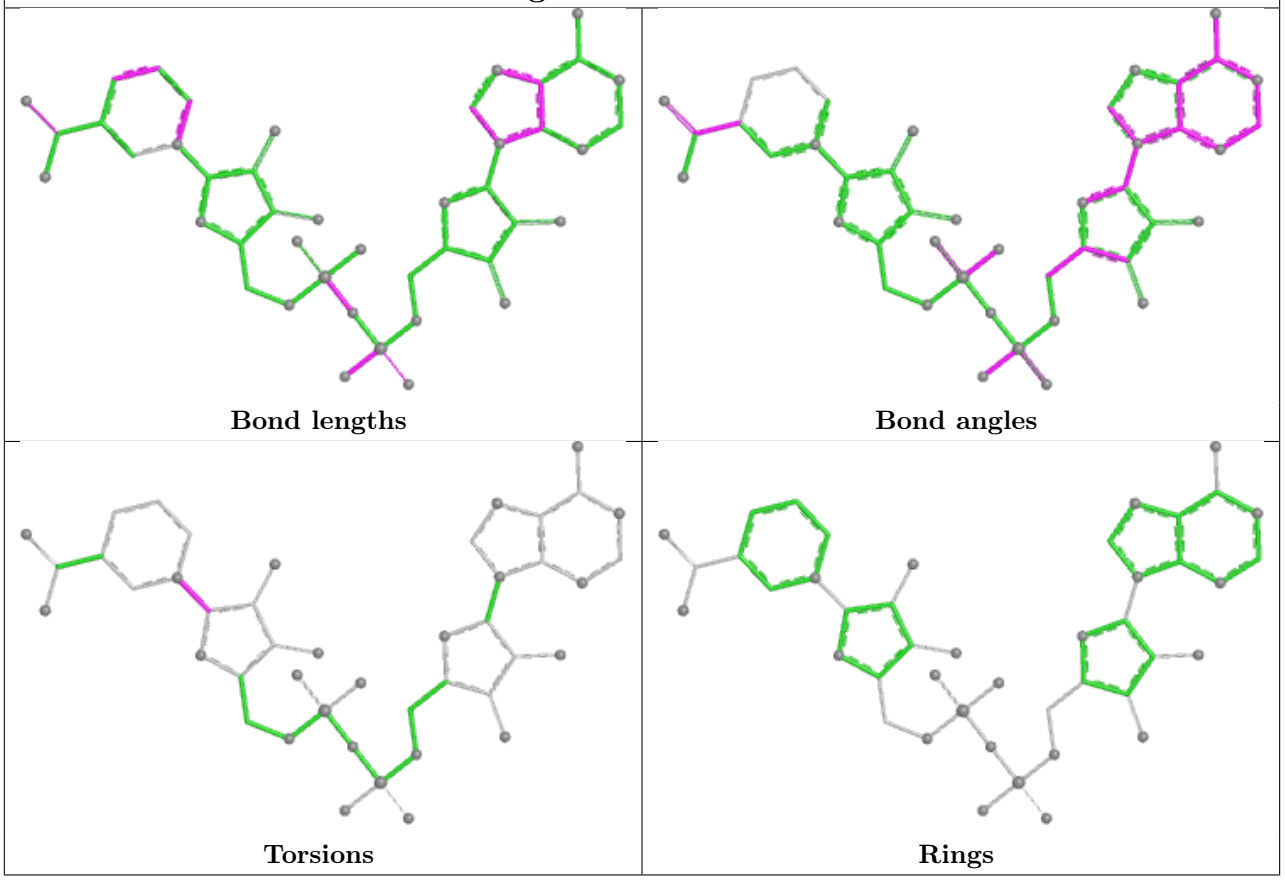


Torsions



Rings

Ligand NAI B 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	366/380 (96%)	-0.27	7 (1%) 66 66	11, 16, 31, 60	0
1	B	367/380 (96%)	-0.14	15 (4%) 41 41	11, 16, 33, 59	0
1	C	366/380 (96%)	-0.03	16 (4%) 39 38	11, 18, 41, 61	0
1	D	362/380 (95%)	-0.22	8 (2%) 62 62	12, 16, 29, 50	0
All	All	1461/1520 (96%)	-0.16	46 (3%) 51 51	11, 17, 34, 61	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	TRP	6.4
1	A	177	TRP	4.6
1	D	175	TRP	4.1
1	D	225	GLY	4.1
1	C	177	TRP	4.0
1	B	180	THR	4.0
1	B	178	ARG	3.8
1	C	124	ALA	3.7
1	C	224	GLN	3.6
1	B	184	GLY	3.5
1	B	373	LEU	3.5
1	D	170	ASP	3.4
1	B	342	LYS	3.4
1	C	178	ARG	3.3
1	C	125	SER	3.2
1	B	176	SER	3.1
1	D	176	SER	3.1
1	D	223	HIS	3.1
1	A	342	LYS	3.1
1	A	125	SER	3.0
1	A	181	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	340	ARG	2.9
1	B	181	ARG	2.8
1	B	182	LYS	2.7
1	B	49	ASP	2.7
1	D	340	ARG	2.7
1	D	167	TYR	2.6
1	C	49	ASP	2.5
1	A	339	GLY	2.5
1	C	126	ASP	2.5
1	B	183	ASP	2.4
1	C	69	GLU	2.3
1	C	181	ARG	2.3
1	B	71	VAL	2.2
1	C	7	ALA	2.2
1	C	223	HIS	2.2
1	C	182	LYS	2.2
1	B	340	ARG	2.2
1	C	341	GLY	2.2
1	C	340	ARG	2.2
1	A	365	GLN	2.1
1	B	175	TRP	2.1
1	C	225	GLY	2.0
1	D	222	PRO	2.0
1	B	179	LEU	2.0
1	C	342	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 oligosaccharides in this entry.

6.4 Ligands (i)

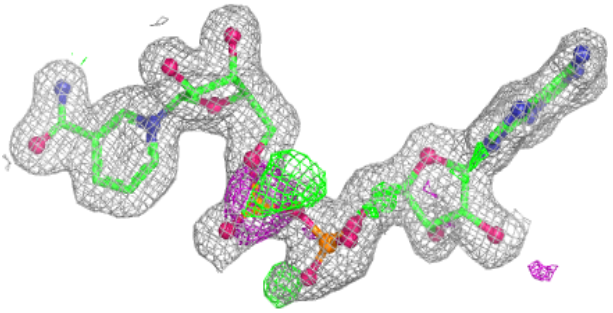
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

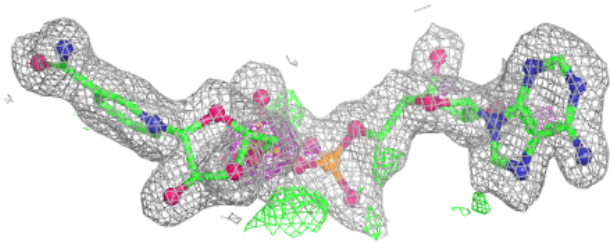
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAI	B	401	44/44	0.91	0.08	16,22,30,33	0
2	NAI	C	401	44/44	0.93	0.08	17,24,26,29	0
3	8S0	C	402	12/12	0.93	0.07	20,21,25,28	0
3	8S0	A	402	12/12	0.95	0.06	18,20,22,25	0
3	8S0	B	402	12/12	0.95	0.06	18,20,24,25	0
2	NAI	A	401	44/44	0.95	0.07	16,19,23,26	0
2	NAI	D	500	44/44	0.97	0.06	14,17,21,22	0

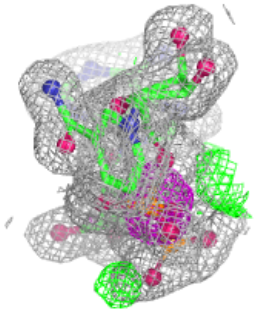
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAI 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)

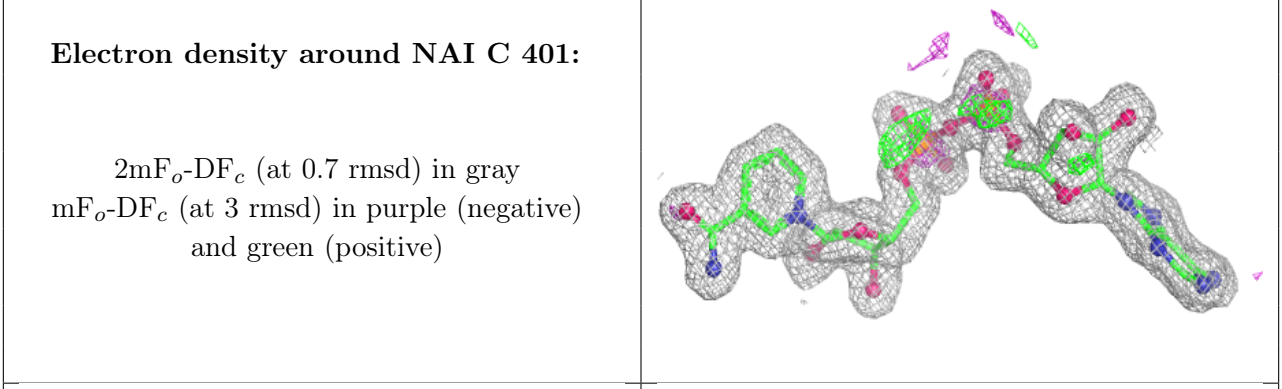






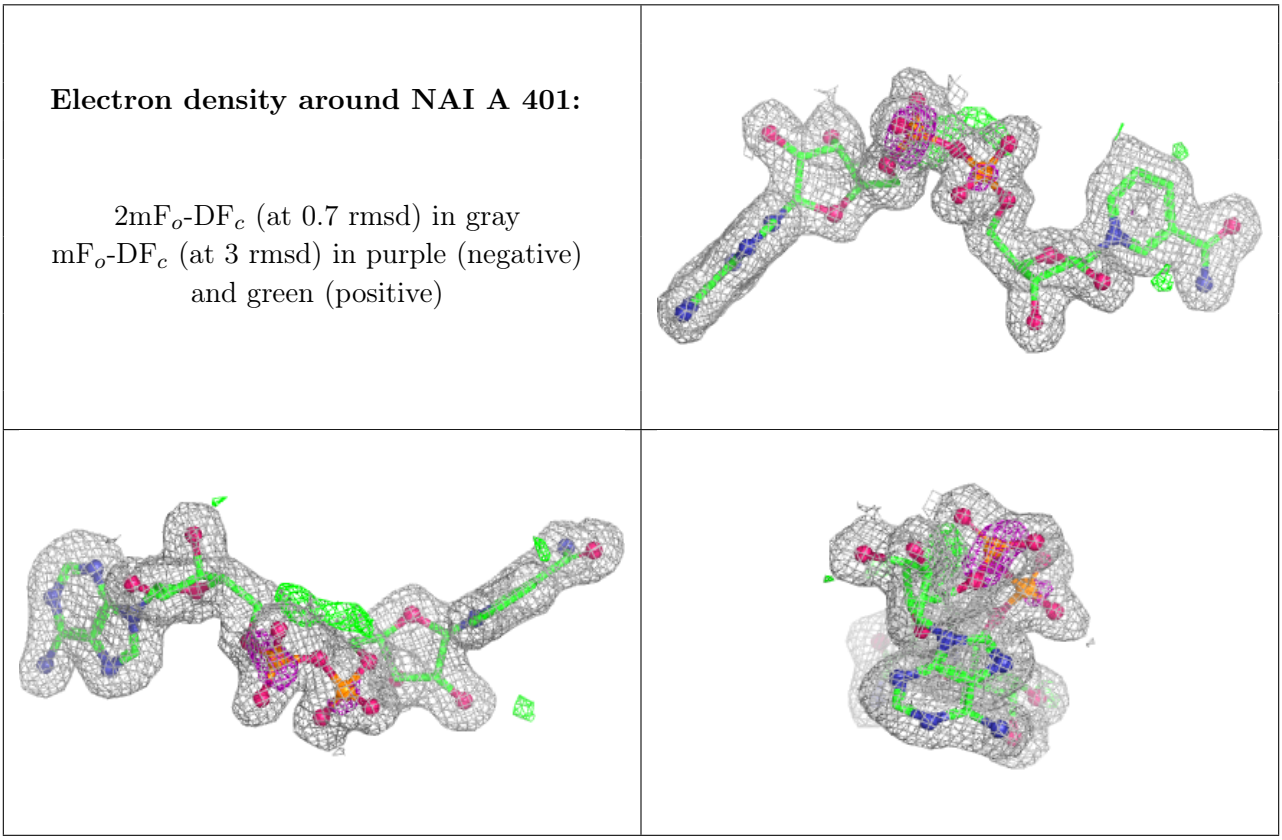
Electron density around NAI C 401:

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



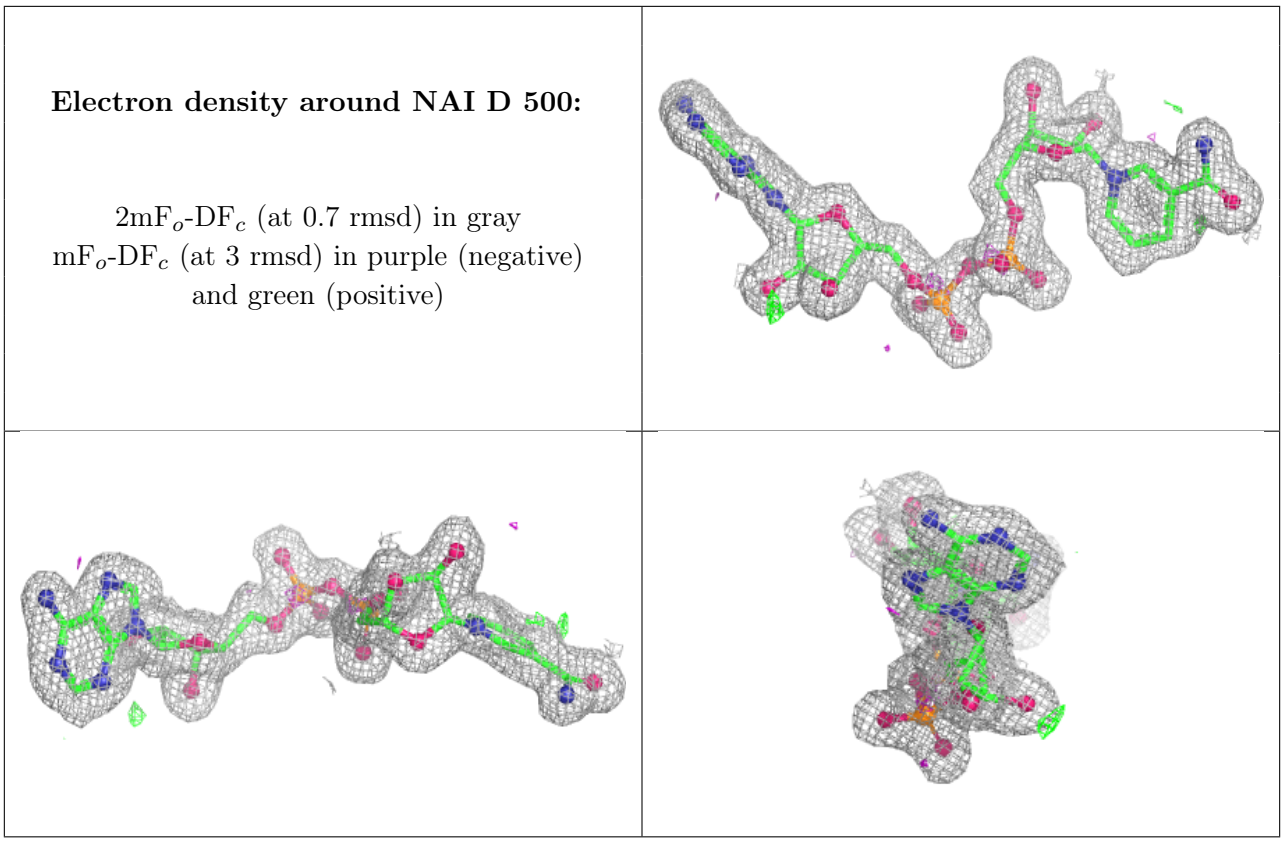
Electron density around NAI A 401:

$2mF_o$-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 D 500:

$2mF_o$-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.