



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:39 PM UTC

PDB ID : 7DL3 / pdb_00007dl3
Title : The structure of 3,5-DAHDHcca complex with NADPH
Authors : Liu, N.; Wu, L.; Zhu, D.M.; Zhou, J.H.
Deposited on : 2020-11-25
Resolution : 1.85 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

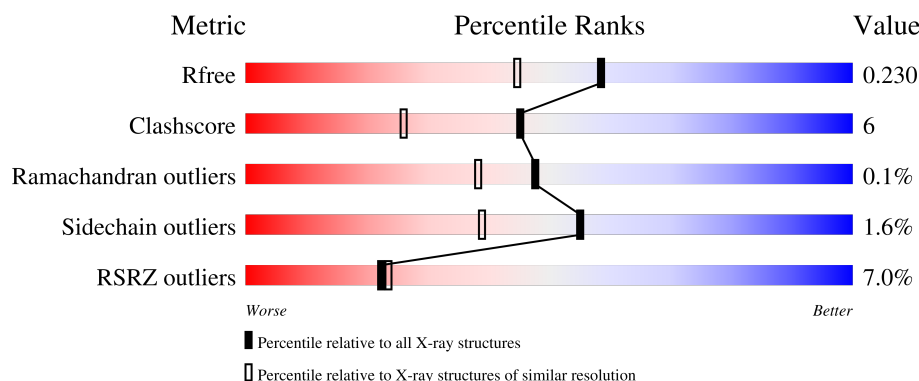
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	358	4% 87% 11% ..
1	B	358	4% 88% 9% ..
1	C	358	6% 85% 13% .
1	D	358	14% 84% 14% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11770 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 3,5-diaminohexanoate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2697	1691	471	517	18			
1	B	351	Total	C	N	O	S	0	1	0
			2674	1678	464	514	18			
1	C	351	Total	C	N	O	S	0	1	0
			2674	1678	465	513	18			
1	D	351	Total	C	N	O	S	0	1	0
			2671	1676	464	513	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	HIS	-	expression tag	UNP B0VJ11
A	354	HIS	-	expression tag	UNP B0VJ11
A	355	HIS	-	expression tag	UNP B0VJ11
A	356	HIS	-	expression tag	UNP B0VJ11
A	357	HIS	-	expression tag	UNP B0VJ11
A	358	HIS	-	expression tag	UNP B0VJ11
B	353	HIS	-	expression tag	UNP B0VJ11
B	354	HIS	-	expression tag	UNP B0VJ11
B	355	HIS	-	expression tag	UNP B0VJ11
B	356	HIS	-	expression tag	UNP B0VJ11
B	357	HIS	-	expression tag	UNP B0VJ11
B	358	HIS	-	expression tag	UNP B0VJ11
C	353	HIS	-	expression tag	UNP B0VJ11
C	354	HIS	-	expression tag	UNP B0VJ11
C	355	HIS	-	expression tag	UNP B0VJ11
C	356	HIS	-	expression tag	UNP B0VJ11
C	357	HIS	-	expression tag	UNP B0VJ11
C	358	HIS	-	expression tag	UNP B0VJ11
D	353	HIS	-	expression tag	UNP B0VJ11
D	354	HIS	-	expression tag	UNP B0VJ11
D	355	HIS	-	expression tag	UNP B0VJ11

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Chain	Residue	Modelled	Actual	Comment	Reference
D	356	HIS	-	expression tag	UNP B0VJ11
D	357	HIS	-	expression tag	UNP B0VJ11
D	358	HIS	-	expression tag	UNP B0VJ11

- # NAP

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4 | A | 268 | Total O
268 268 | 0 | 0 |



WORLD WIDE
PDB
PROTEIN DATA BANK

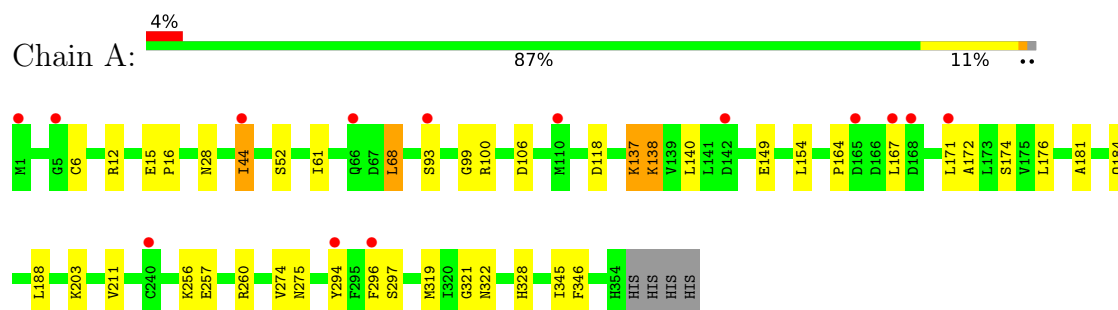
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	217	Total 217	O 217	0	0
4	C	237	Total 237	O 237	0	0
4	D	234	Total 234	O 234	0	0

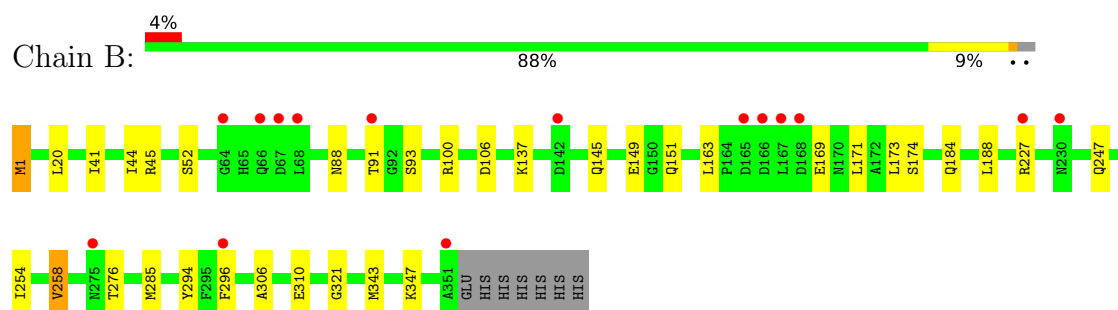
3 Residue-property plots [i](#)

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.

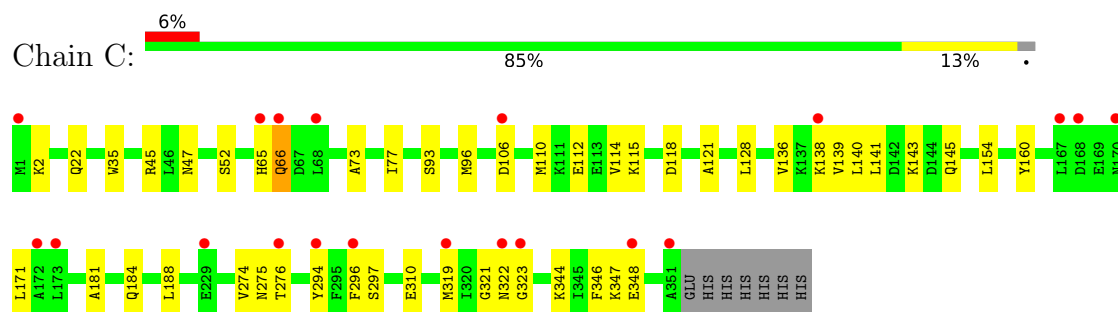
- Molecule 1: 3,5-diaminohexanoate dehydrogenase



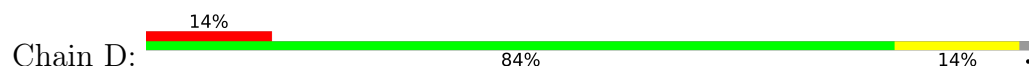
- Molecule 1: 3,5-diaminohexanoate dehydrogenase

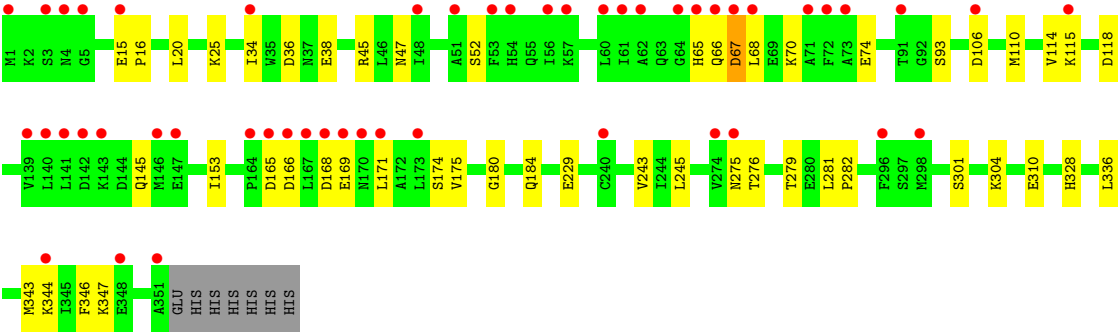


- Molecule 1: 3,5-diaminohexanoate dehydrogenase



- Molecule 1: 3,5-diaminohexanoate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.59Å 122.04Å 114.64Å 90.00° 94.85° 90.00°	Depositor
Resolution (Å)	47.72 – 1.85 47.72 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.72-1.85) 96.9 (47.72-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.201 , 0.229 0.202 , 0.230	Depositor DCC
R_{free} test set	6325 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11770	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2732	0.61	0/3681
1	B	0.35	0/2710	0.60	0/3651
1	C	0.38	0/2710	0.63	0/3651
1	D	0.37	0/2707	0.70	6/3647 (0.2%)
All	All	0.37	0/10859	0.64	6/14630 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	67	ASP	N-CA-C	-8.26	93.21	110.80
1	D	66	GLN	CA-C-N	7.63	136.11	121.54
1	D	66	GLN	C-N-CA	7.63	136.11	121.54
1	D	165	ASP	CA-C-N	5.61	128.36	120.28
1	D	165	ASP	C-N-CA	5.61	128.36	120.28
1	D	67	ASP	N-CA-CB	5.18	119.25	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	166	ASP	Peptide
1	D	65	HIS	Peptide

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	2697	0	2753	30	0
1	B	2674	0	2739	27	0
1	C	2674	0	2741	45	0
1	D	2671	0	2738	29	0
2	A	48	0	25	2	0
2	C	48	0	25	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	268	0	0	5	0
4	B	217	0	0	1	0
4	C	237	0	0	4	0
4	D	234	0	0	3	0
All	All	11770	0	11021	128	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 6.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:MET:HG3	1:D:347:LYS:HE2	1.41	1.01
1:D:45:ARG:NH1	1:D:169:GLU:OE2	2.04	0.89
1:B:91:THR:HG23	1:B:93:SER:H	1.39	0.88
1:C:110:MET:HE1	1:C:114:VAL:HG22	1.59	0.83
1:A:6:CYS:SG	4:A:753:HOH:O	2.36	0.82
1:A:188:LEU:HD11	1:A:294:TYR:CD1	2.15	0.80
1:C:294:TYR:CE1	1:C:321:GLY:HA2	2.18	0.79
1:A:257:GLU:OE2	1:A:260:ARG:NH2	2.16	0.78
1:A:294:TYR:CE2	1:A:321:GLY:HA2	2.20	0.77
1:D:175:VAL:HG21	1:D:336:LEU:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:O	4:A:501:HOH:O	2.07	0.72
1:C:77:ILE:HD11	1:C:136:VAL:HG23	1.75	0.68
1:C:276:THR:OG1	2:C:401:NAP:N7A	2.26	0.68
1:B:227:ARG:HE	1:B:247:GLN:HG2	1.59	0.68
1:C:344:LYS:O	1:C:348:GLU:HG3	1.94	0.68
1:A:106:ASP:OD2	4:A:502:HOH:O	2.12	0.67
1:C:184[A]:GLN:OE1	4:C:501:HOH:O	2.10	0.67
1:D:15:GLU:OE1	1:D:25:LYS:HB2	1.94	0.67
1:A:171:LEU:HD21	1:A:346:PHE:HB3	1.77	0.66
1:C:184[A]:GLN:HB3	1:C:294:TYR:HE2	1.60	0.66
1:A:188:LEU:HD11	1:A:294:TYR:HD1	1.59	0.66
1:A:184:GLN:HB3	1:A:294:TYR:HE1	1.61	0.65
1:C:188:LEU:HD11	1:C:294:TYR:CD2	2.31	0.65
1:A:137:LYS:HD2	1:A:149:GLU:HG3	1.79	0.65
1:C:184[A]:GLN:NE2	4:C:505:HOH:O	2.28	0.65
1:D:34:ILE:HD12	1:D:153:ILE:HD11	1.78	0.64
1:C:274:VAL:O	1:C:297:SER:HB2	1.99	0.62
1:A:275:ASN:OD1	2:A:401:NAP:H8A	1.99	0.62
1:C:184[A]:GLN:HB3	1:C:294:TYR:CE2	2.37	0.60
1:B:254:ILE:O	1:B:258:VAL:HG13	2.03	0.59
1:A:257:GLU:CD	1:A:260:ARG:HH21	2.09	0.59
1:B:88:ASN:HB3	1:B:91:THR:HG22	1.84	0.58
1:D:175:VAL:HG21	1:D:336:LEU:CD1	2.34	0.57
1:A:319:MET:HE1	1:C:319:MET:HB2	1.86	0.57
1:D:229:GLU:HA	1:D:245:LEU:HD21	1.87	0.57
1:B:88:ASN:CG	1:B:91:THR:HG22	2.29	0.57
1:D:275:ASN:ND2	4:D:407:HOH:O	2.38	0.56
1:C:184[B]:GLN:HB3	1:C:294:TYR:HE2	1.70	0.56
1:D:171:LEU:HD11	1:D:346:PHE:HB3	1.88	0.56
1:C:52:SER:HB2	1:C:93:SER:HB2	1.88	0.56
1:B:227:ARG:HH11	1:B:247:GLN:CD	2.14	0.55
1:C:294:TYR:HE1	1:C:321:GLY:HA2	1.69	0.55
1:D:171:LEU:O	1:D:174:SER:OG	2.23	0.55
1:A:164:PRO:HG2	1:A:167:LEU:HD12	1.89	0.54
1:B:169:GLU:O	1:B:173:LEU:HD23	2.07	0.53
1:D:310:GLU:OE2	4:D:401:HOH:O	2.19	0.53
1:C:184[B]:GLN:HE22	1:C:323:GLY:H	1.56	0.53
1:D:175:VAL:CG2	1:D:336:LEU:HD11	2.36	0.53
1:C:184[B]:GLN:NE2	1:C:322:ASN:HB3	2.23	0.52
1:D:36:ASP:HB2	1:D:106:ASP:OD1	2.09	0.52
1:A:294:TYR:HE2	1:A:321:GLY:HA2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:HD23	1:C:143:LYS:HD2	1.91	0.52
1:C:275:ASN:OD1	2:C:401:NAP:H8A	2.10	0.52
1:B:171:LEU:CD1	1:B:347:LYS:HG2	2.40	0.52
1:B:137:LYS:HE2	1:B:149:GLU:HG2	1.92	0.51
1:B:171:LEU:HD12	1:B:347:LYS:HG2	1.92	0.51
1:A:274:VAL:O	1:A:297:SER:HB2	2.11	0.51
1:C:65:HIS:O	1:C:66:GLN:HB3	2.11	0.51
1:B:343:MET:HG3	1:B:347:LYS:HE2	1.92	0.51
1:A:184:GLN:HB3	1:A:294:TYR:CE1	2.45	0.51
1:C:110:MET:HE2	1:C:112:GLU:O	2.11	0.51
1:C:184[B]:GLN:HE22	1:C:322:ASN:HB3	1.76	0.50
1:B:45:ARG:HD2	1:B:145:GLN:CD	2.36	0.50
1:C:310:GLU:OE1	4:C:502:HOH:O	2.19	0.50
1:D:34:ILE:HG22	1:D:38:GLU:HB2	1.94	0.50
1:B:88:ASN:CB	1:B:91:THR:HG22	2.42	0.50
1:B:171:LEU:O	1:B:174:SER:OG	2.30	0.49
1:B:184:GLN:HB2	1:B:296:PHE:HZ	1.77	0.49
1:C:184[B]:GLN:HB3	1:C:294:TYR:CE2	2.47	0.49
1:C:181:ALA:HB2	2:C:401:NAP:H5N	1.94	0.49
1:C:184[B]:GLN:HB2	1:C:296:PHE:HZ	1.78	0.49
1:C:73:ALA:O	1:C:77:ILE:HD13	2.12	0.49
1:C:96:MET:HE1	1:C:121:ALA:HB1	1.95	0.49
1:C:184[A]:GLN:HB2	1:C:296:PHE:HZ	1.77	0.48
1:D:115:LYS:HD3	1:D:118:ASP:OD2	2.13	0.48
1:B:52:SER:HB2	1:B:93:SER:HB3	1.95	0.48
1:B:306:ALA:O	1:B:310:GLU:HG3	2.13	0.48
1:C:181:ALA:HA	1:C:296:PHE:CZ	2.49	0.48
1:A:44:ILE:HG12	1:A:99:GLY:HA2	1.95	0.48
1:D:47:ASN:OD1	1:D:145:GLN:HG2	2.13	0.47
1:A:181:ALA:HA	1:A:296:PHE:CZ	2.49	0.47
1:B:20:LEU:HD13	1:D:281:LEU:HD13	1.97	0.46
1:C:138:LYS:NZ	1:C:139:VAL:O	2.43	0.46
1:A:61:ILE:CG1	1:A:68:LEU:HD11	2.45	0.46
1:A:138:LYS:HG3	1:A:140:LEU:CD1	2.47	0.45
1:A:184:GLN:OE1	4:A:503:HOH:O	2.20	0.45
1:B:45:ARG:NH2	1:B:169:GLU:OE1	2.50	0.45
1:B:1:MET:HE1	1:B:106:ASP:H	1.81	0.45
1:B:294:TYR:CE1	1:B:321:GLY:HA2	2.52	0.45
1:C:110:MET:CE	1:C:114:VAL:HG22	2.40	0.45
1:D:344:LYS:HA	1:D:347:LYS:HE3	1.99	0.45
1:A:174:SER:O	1:A:203:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASP:N	1:C:106:ASP:OD1	2.50	0.44
1:C:297:SER:HB3	4:C:518:HOH:O	2.17	0.44
1:B:285:MET:SD	1:D:20:LEU:HD11	2.58	0.44
1:C:47:ASN:OD1	1:C:145:GLN:HG2	2.17	0.44
1:C:294:TYR:CE1	1:C:319:MET:HG2	2.53	0.44
1:D:344:LYS:NZ	4:D:403:HOH:O	2.29	0.44
1:C:171:LEU:HD12	1:C:347:LYS:HA	2.00	0.44
1:A:12:ARG:HD3	1:A:28:ASN:O	2.18	0.44
1:A:345:ILE:HA	4:A:507:HOH:O	2.18	0.44
1:C:45:ARG:CZ	1:C:45:ARG:HB2	2.48	0.43
1:C:184[B]:GLN:HE22	1:C:323:GLY:N	2.16	0.43
1:B:41:ILE:O	1:B:151:GLN:HA	2.19	0.43
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.85	0.43
1:B:169:GLU:HA	4:B:509:HOH:O	2.19	0.43
1:D:34:ILE:CG2	1:D:38:GLU:HB2	2.48	0.43
1:C:140:LEU:CD2	1:C:143:LYS:HD2	2.48	0.43
1:D:15:GLU:HA	1:D:16:PRO:HA	1.80	0.43
1:D:180:GLY:O	1:D:184:GLN:HG2	2.18	0.43
1:B:44:ILE:HD11	1:B:100:ARG:HG3	2.01	0.42
1:D:110:MET:HE1	1:D:114:VAL:O	2.20	0.42
1:A:52:SER:HB2	1:A:93:SER:HB2	2.02	0.42
1:D:168:ASP:O	1:D:171:LEU:HB3	2.20	0.42
1:D:70:LYS:HE3	1:D:74:GLU:OE1	2.19	0.42
1:D:52:SER:HB2	1:D:93:SER:OG	2.19	0.42
1:C:45:ARG:HB2	1:C:45:ARG:NH1	2.35	0.41
1:A:181:ALA:HB2	2:A:401:NAP:H5N	2.01	0.41
1:A:15:GLU:HA	1:A:16:PRO:HA	1.90	0.41
1:C:110:MET:HE3	1:C:160:TYR:OH	2.21	0.41
1:C:22:GLN:HB2	1:C:128:LEU:HB3	2.03	0.41
1:C:115:LYS:HD3	1:C:118:ASP:OD2	2.21	0.41
1:B:188:LEU:HD11	1:B:294:TYR:CD2	2.55	0.40
1:A:100:ARG:HA	1:A:118:ASP:O	2.21	0.40
1:C:2:LYS:HE2	1:C:35:TRP:CZ2	2.56	0.40
1:D:279:THR:C	1:D:282:PRO:HD2	2.47	0.40
1:A:172:ALA:O	1:A:176:LEU:HG	2.22	0.40
1:D:301:SER:HB3	1:D:304:LYS:HB2	2.04	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	352/358 (98%)	347 (99%)	5 (1%)	0	100	100
1	B	350/358 (98%)	346 (99%)	4 (1%)	0	100	100
1	C	350/358 (98%)	343 (98%)	6 (2%)	1 (0%)	36	25
1	D	350/358 (98%)	343 (98%)	6 (2%)	1 (0%)	36	25
All	All	1402/1432 (98%)	1379 (98%)	21 (2%)	2 (0%)	48	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	67	ASP
1	C	66	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	292/296 (99%)	284 (97%)	8 (3%)	39	22
1	B	290/296 (98%)	287 (99%)	3 (1%)	68	58
1	C	290/296 (98%)	287 (99%)	3 (1%)	68	58
1	D	290/296 (98%)	286 (99%)	4 (1%)	59	45
All	All	1162/1184 (98%)	1144 (98%)	18 (2%)	55	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	68	LEU
1	A	137	LYS
1	A	138	LYS
1	A	154	LEU
1	A	211	VAL
1	A	256	LYS
1	A	328	HIS
1	B	1	MET
1	B	258	VAL
1	B	276	THR
1	C	141	LEU
1	C	154	LEU
1	C	346	PHE
1	D	68	LEU
1	D	243	VAL
1	D	276	THR
1	D	328	HIS

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

Mol	Chain	Res	Type
1	A	58	ASN
1	A	354	HIS
1	B	22	GLN
1	B	63	GLN
1	B	247	GLN
1	C	63	GLN
1	C	134	ASN
1	D	54	HIS
1	D	230	ASN
1	D	275	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	A	401	-	50,52,52	1.15	6 (12%)	71,80,80	1.46	10 (14%)
2	NAP	C	401	-	50,52,52	1.25	6 (12%)	71,80,80	1.60	13 (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
2	NAP	A	401	-	-	4/35/67/67	0/5/5/5
2	NAP	C	401	-	-	6/35/67/67	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C5A-C4A	4.34	1.46	1.39
2	C	401	NAP	C5A-C4A	4.05	1.46	1.39
2	C	401	NAP	PN-O3	3.33	1.63	1.59
2	C	401	NAP	PA-O3	2.74	1.62	1.59
2	A	401	NAP	PN-O3	2.44	1.62	1.59
2	C	401	NAP	C5A-C6A	2.38	1.47	1.41
2	C	401	NAP	C5A-N7A	-2.34	1.34	1.39
2	A	401	NAP	C5A-C6A	2.33	1.47	1.41
2	A	401	NAP	PA-O3	2.25	1.61	1.59
2	C	401	NAP	C4A-N9A	-2.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O4D-C1D	2.07	1.43	1.40
2	A	401	NAP	C5A-N7A	-2.01	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAP	C5A-C4A-N3A	-5.12	119.66	126.72
2	A	401	NAP	C5A-C4A-N3A	-4.81	120.09	126.72
2	C	401	NAP	N3A-C4A-N9A	4.22	134.35	127.17
2	A	401	NAP	N3A-C4A-N9A	4.13	134.19	127.17
2	C	401	NAP	C4A-C5A-N7A	-3.72	106.33	110.58
2	C	401	NAP	N3A-C2A-N1A	-3.63	123.08	128.58
2	C	401	NAP	C2A-N3A-C4A	3.56	120.53	111.83
2	C	401	NAP	C4A-N9A-C8A	3.35	109.26	105.74
2	A	401	NAP	C4A-N9A-C8A	3.30	109.20	105.74
2	A	401	NAP	C2A-N3A-C4A	3.25	119.76	111.83
2	A	401	NAP	N3A-C2A-N1A	-3.21	123.72	128.58
2	A	401	NAP	C4A-C5A-N7A	-3.17	106.96	110.58
2	C	401	NAP	C5A-N7A-C8A	2.88	107.97	103.45
2	C	401	NAP	C2N-N1N-C1D	-2.70	113.16	119.13
2	A	401	NAP	C5A-N7A-C8A	2.57	107.49	103.45
2	C	401	NAP	C6A-C5A-N7A	2.53	136.96	132.09
2	C	401	NAP	N9A-C8A-N7A	-2.46	110.45	113.94
2	A	401	NAP	C6A-C5A-N7A	2.36	136.63	132.09
2	A	401	NAP	O2N-PN-O3	2.33	113.56	107.27
2	A	401	NAP	N9A-C8A-N7A	-2.32	110.65	113.94
2	C	401	NAP	C6N-N1N-C1D	2.21	124.07	119.73
2	C	401	NAP	C2A-N1A-C6A	2.11	122.20	118.73
2	C	401	NAP	O3D-C3D-C2D	-2.06	105.23	111.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	NAP	C2N-C3N-C7N-O7N
2	C	401	NAP	C2N-C3N-C7N-N7N
2	C	401	NAP	C4N-C3N-C7N-O7N
2	C	401	NAP	C4N-C3N-C7N-N7N
2	A	401	NAP	C2N-C3N-C7N-O7N
2	A	401	NAP	C4N-C3N-C7N-O7N
2	A	401	NAP	C4N-C3N-C7N-N7N
2	A	401	NAP	C2N-C3N-C7N-N7N

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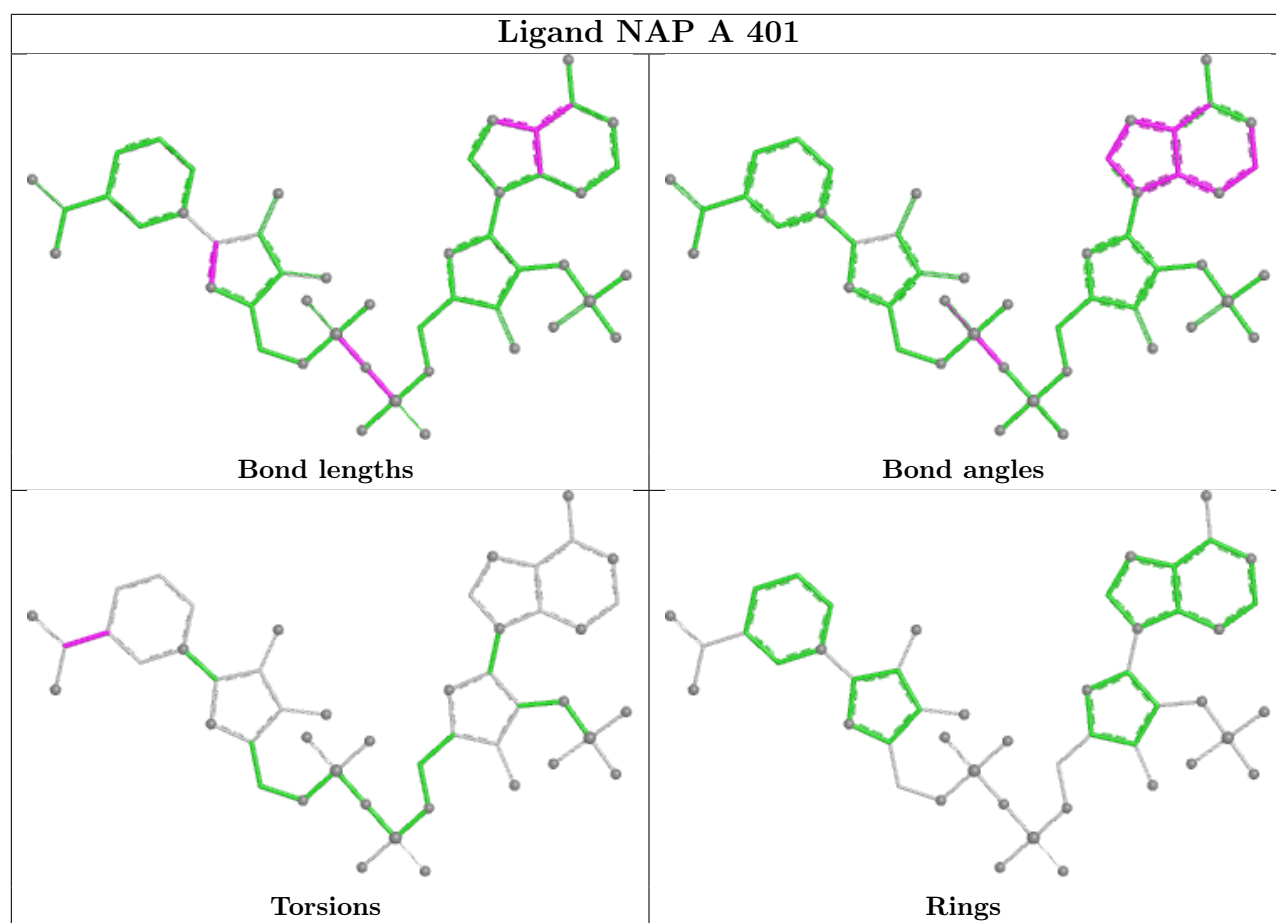
Mol	Chain	Res	Type	Atoms
2	C	401	NAP	C5D-O5D-PN-O1N
2	C	401	NAP	O4B-C4B-C5B-O5B

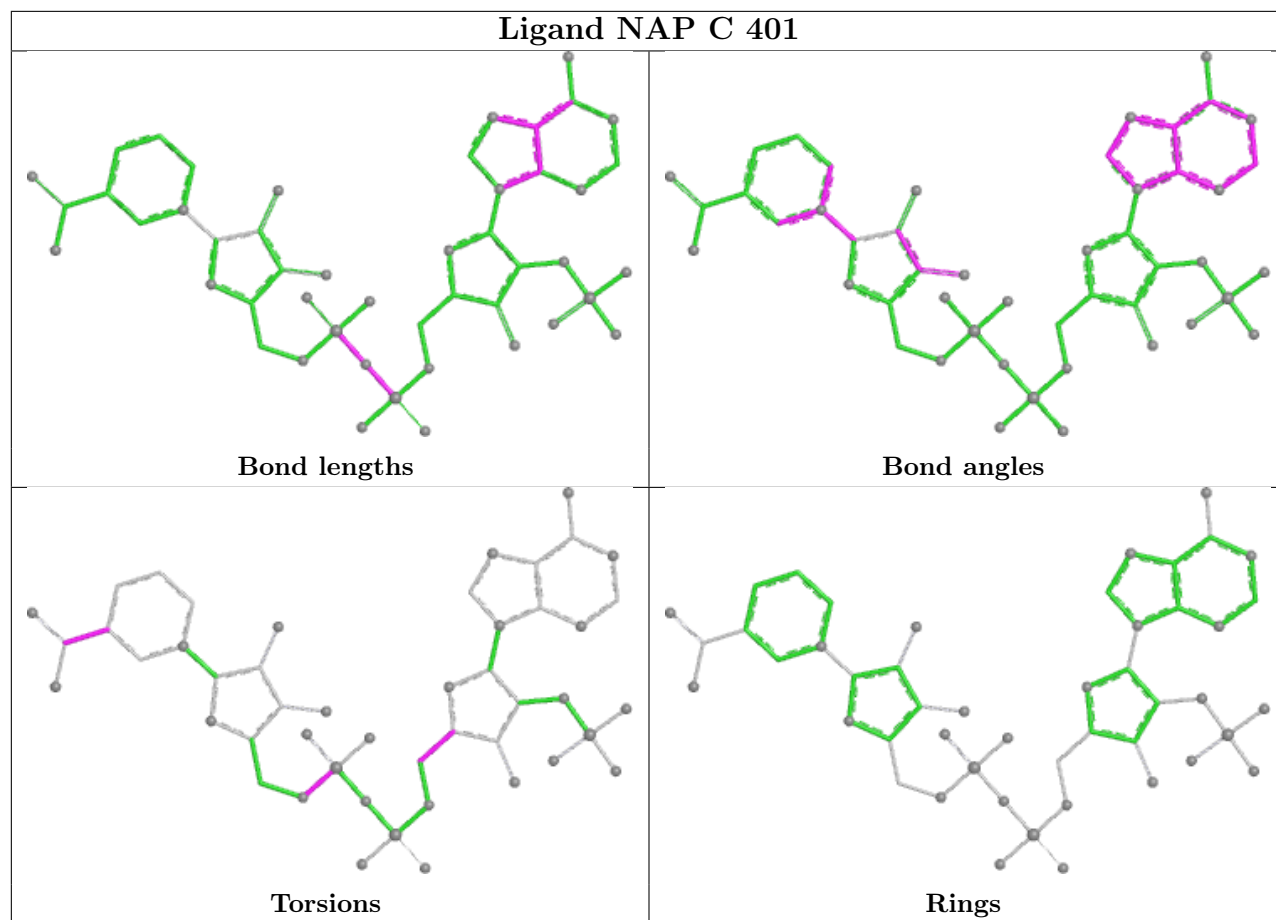
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	2	0
2	C	401	NAP	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	354/358 (98%)	0.08	14 (3%) 42 45	10, 18, 34, 52	0
1	B	351/358 (98%)	0.28	15 (4%) 40 42	11, 21, 39, 62	1 (0%)
1	C	351/358 (98%)	0.23	20 (5%) 29 31	9, 19, 38, 57	2 (0%)
1	D	351/358 (98%)	0.56	50 (14%) 6 6	9, 21, 47, 62	1 (0%)
All	All	1407/1432 (98%)	0.29	99 (7%) 22 23	9, 20, 42, 62	4 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	TYR	7.5
1	C	351	ALA	5.8
1	B	351	ALA	5.1
1	A	294	TYR	5.0
1	D	351	ALA	5.0
1	B	227	ARG	4.8
1	D	165	ASP	4.6
1	C	167	LEU	4.5
1	D	240	CYS	4.5
1	D	66	GLN	4.4
1	A	110	MET	4.3
1	D	68	LEU	4.3
1	D	4	ASN	4.2
1	D	61	ILE	4.1
1	D	67	ASP	3.9
1	D	167	LEU	3.9
1	D	62	ALA	3.8
1	D	34	ILE	3.8
1	D	71	ALA	3.7
1	B	167	LEU	3.7
1	D	56	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	64	GLY	3.6
1	D	72	PHE	3.6
1	D	166	ASP	3.6
1	D	140	LEU	3.6
1	C	68	LEU	3.5
1	C	296	PHE	3.5
1	D	173	LEU	3.5
1	D	139	VAL	3.5
1	A	1	MET	3.5
1	C	323	GLY	3.5
1	C	168	ASP	3.4
1	D	141	LEU	3.4
1	D	65	HIS	3.3
1	D	106	ASP	3.3
1	D	168	ASP	3.3
1	C	106	ASP	3.2
1	D	60	LEU	3.2
1	C	66	GLN	3.0
1	C	1	MET	3.0
1	D	57	LYS	2.9
1	A	167	LEU	2.9
1	D	275	ASN	2.9
1	D	142	ASP	2.8
1	B	68	LEU	2.7
1	A	240	CYS	2.7
1	C	348	GLU	2.7
1	D	15	GLU	2.7
1	D	73	ALA	2.6
1	D	115	LYS	2.6
1	C	170	ASN	2.6
1	B	64	GLY	2.6
1	B	168	ASP	2.6
1	A	296	PHE	2.6
1	A	171	LEU	2.6
1	D	5	GLY	2.6
1	B	166	ASP	2.6
1	D	1	MET	2.5
1	D	298	MET	2.5
1	C	138	LYS	2.5
1	C	322	ASN	2.5
1	D	54	HIS	2.5
1	C	319	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLN	2.4
1	D	48	ILE	2.4
1	D	170	ASN	2.4
1	D	296	PHE	2.4
1	D	51	ALA	2.4
1	B	91	THR	2.4
1	C	276	THR	2.4
1	D	146	MET	2.4
1	A	168	ASP	2.3
1	B	165	ASP	2.3
1	D	3	SER	2.3
1	D	169	GLU	2.3
1	C	65	HIS	2.3
1	C	172	ALA	2.2
1	C	229	GLU	2.2
1	D	53	PHE	2.2
1	A	93	SER	2.2
1	D	274	VAL	2.2
1	D	147	GLU	2.2
1	A	44	ILE	2.2
1	D	171	LEU	2.2
1	B	230	ASN	2.2
1	D	344	LYS	2.2
1	A	142	ASP	2.1
1	A	165	ASP	2.1
1	D	143	LYS	2.1
1	D	348	GLU	2.1
1	B	296	PHE	2.1
1	B	67	ASP	2.1
1	D	164	PRO	2.1
1	B	275	ASN	2.1
1	C	173	LEU	2.1
1	B	142	ASP	2.1
1	B	66	GLN	2.1
1	D	91	THR	2.0
1	A	5	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

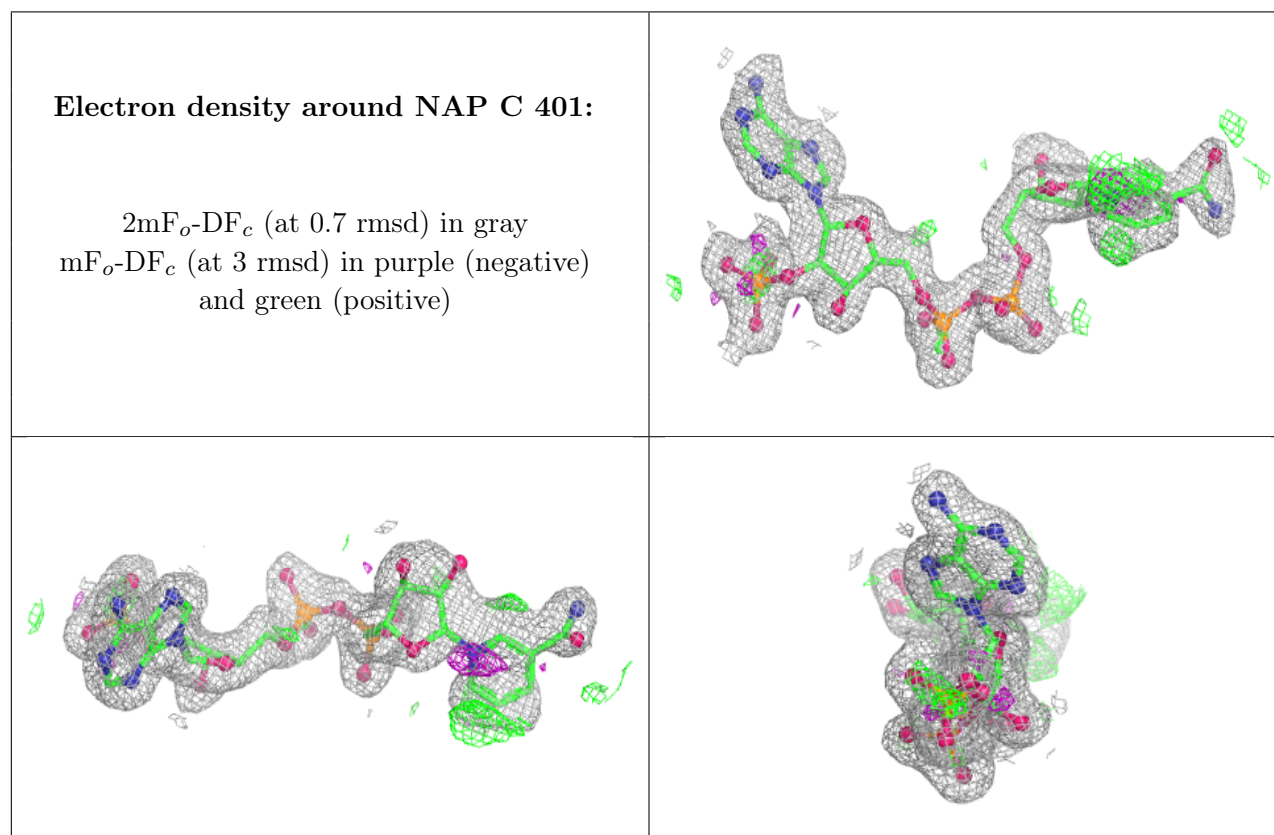
There are no oligosaccharides in this entry.

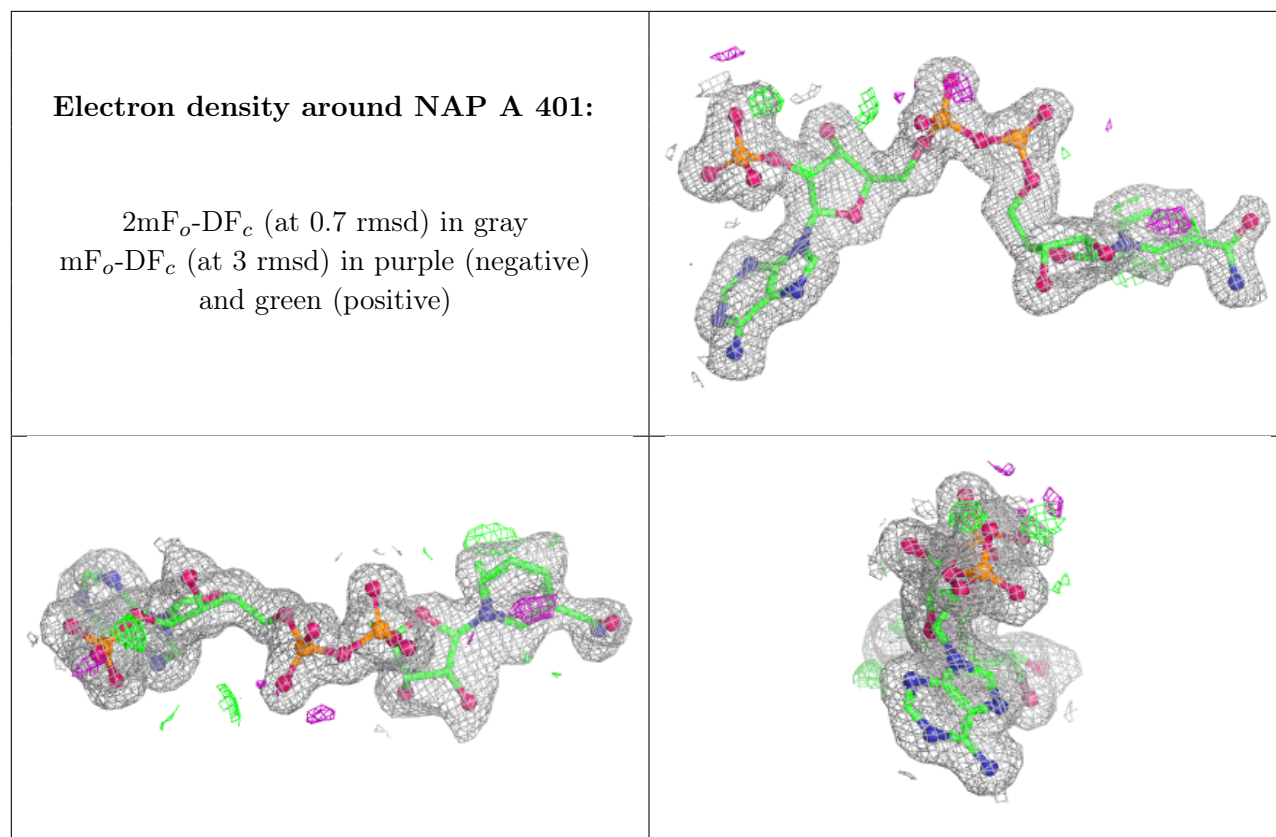
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	NAP	C	401	48/48	0.90	0.12	18,31,42,45	0
3	CL	C	402	1/1	0.95	0.08	39,39,39,39	0
2	NAP	A	401	48/48	0.96	0.08	13,19,37,40	0
3	CL	A	402	1/1	0.99	0.08	26,26,26,26	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.