



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:45 PM UTC

PDB ID : 1UXU / pdb_00001uxu
Title : Structural basis for allosteric regulation and substrate specificity of the non-phosphorylating glyceraldehyde-3-phosphate dehydrogenase (GAPN) from *Thermoproteus tenax*
Authors : Lorentzen, E.; Hensel, R.; Pohl, E.
Deposited on : 2004-03-01
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

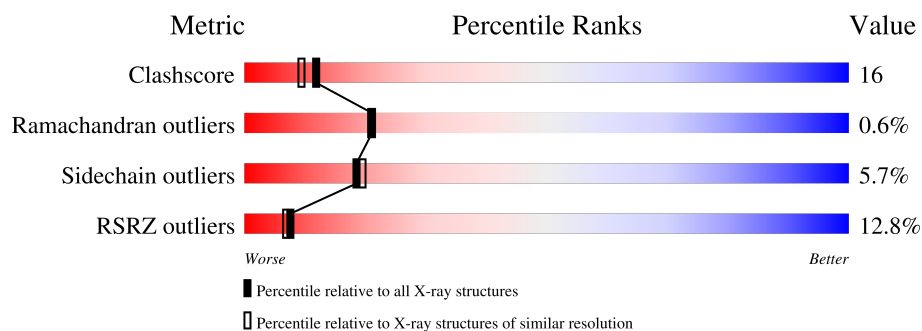
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	501	13% 70% 27% .

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.

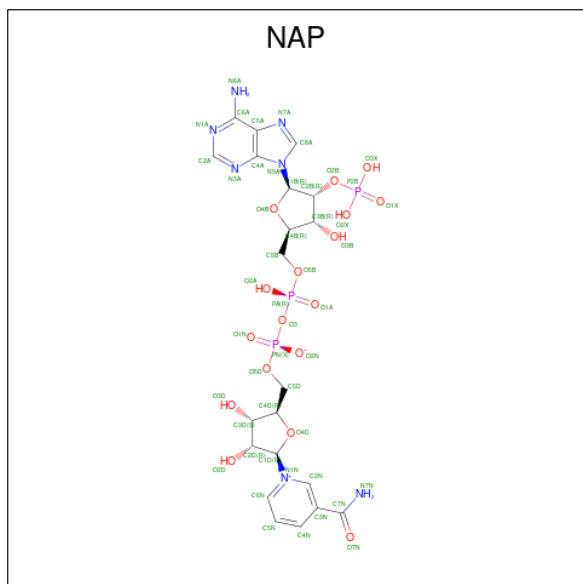
- Molecule 1 is a protein called GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (NADP⁺).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3777	2416	649	703	9			

There are 2 discrepancies between the modelled and reference sequences:

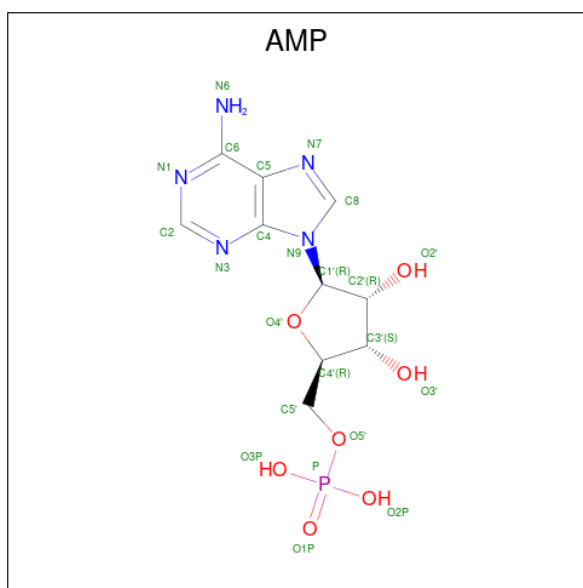
Chain	Residue	Modelled	Actual	Comment	Reference
A	378	PHE	LEU	engineered mutation	UNP O57693
A	402	LEU	SER	conflict	UNP O57693

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



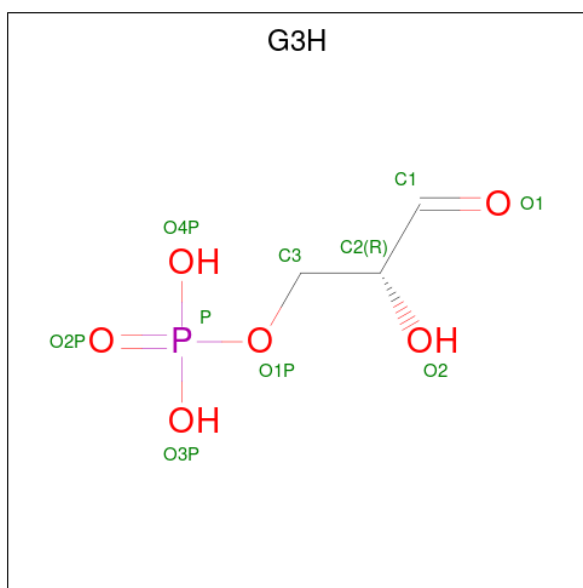
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 15	N 5	O 16	P 3	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is GLYCERALDEHYDE-3-PHOSPHATE (CCD ID: G3H) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0

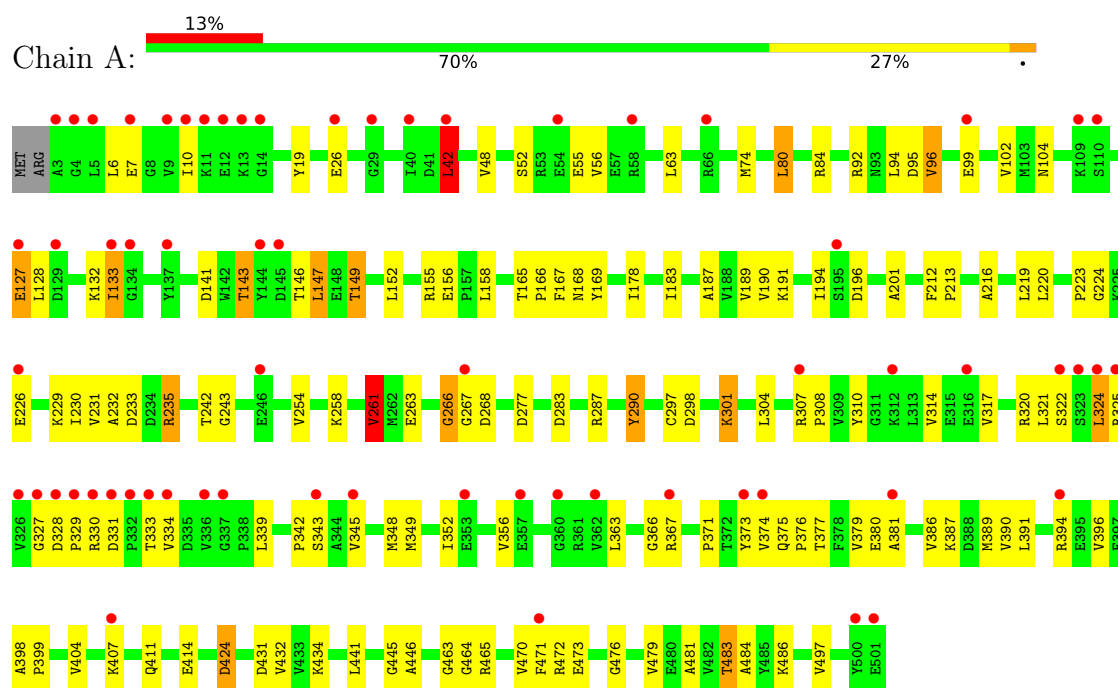
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total 287	O 287	0	0

3 Residue-property plots

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

- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (NADP+)



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	185.29Å 185.29Å 131.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.25 30.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.0 (30.00-2.25) 91.7 (30.00-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.262 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	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	0.95	EDS
Total number of atoms	4137	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: NA, AMP, NAP, G3H

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	0.59	0/3847	1.06	21/5219 (0.4%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	GLY	N-CA-C	-9.90	98.31	112.17
1	A	266	GLY	CA-C-N	-7.93	114.42	122.27
1	A	266	GLY	C-N-CA	-7.93	114.42	122.27
1	A	187	ALA	N-CA-C	-7.80	98.32	110.42
1	A	465	ARG	N-CA-C	-6.72	99.10	109.52
1	A	497	VAL	N-CA-C	-6.67	104.35	110.82
1	A	377	THR	N-CA-C	6.57	120.17	109.59
1	A	261	VAL	N-CA-C	-6.51	98.07	107.78
1	A	473	GLU	N-CA-C	-6.43	100.17	110.14
1	A	290	TYR	N-CA-C	6.38	121.35	113.50
1	A	277	ASP	N-CA-C	-6.07	99.26	108.67
1	A	432	VAL	N-CA-C	6.01	116.75	110.62
1	A	196	ASP	CA-C-N	5.86	126.37	120.04
1	A	196	ASP	C-N-CA	5.86	126.37	120.04
1	A	56	VAL	N-CA-C	-5.83	105.05	110.53
1	A	464	GLY	N-CA-C	5.81	122.45	112.51
1	A	168	ASN	N-CA-C	5.73	119.53	112.54
1	A	74	MET	N-CA-C	-5.73	101.28	109.24
1	A	379	VAL	N-CA-C	5.39	115.86	107.99
1	A	441	LEU	N-CA-C	5.30	119.81	113.23
1	A	242	THR	N-CA-C	-5.09	99.98	108.34

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	3777	0	3857	122	0
2	A	39	0	18	2	0
3	A	23	0	12	6	0
4	A	10	0	5	3	0
5	A	1	0	0	0	0
6	A	287	0	0	12	0
All	All	4137	0	3892	122	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 16.

All (122) 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:267:GLY:HA3	1:A:301:LYS:HG3	1.43	0.96
1:A:386:VAL:HA	1:A:389:MET:HE2	1.51	0.92
1:A:243:GLY:HA2	2:A:502:NAP:H52N	1.59	0.84
1:A:233:ASP:OD1	1:A:235:ARG:HD3	1.79	0.82
1:A:261:VAL:HG22	1:A:481:ALA:HB1	1.64	0.80
1:A:381:ALA:CB	1:A:389:MET:HE1	2.16	0.75
1:A:220:LEU:HD12	1:A:230:ILE:HD11	1.67	0.74
1:A:146:THR:O	1:A:149:THR:HB	1.86	0.74
1:A:155:ARG:HD3	1:A:483:THR:HG21	1.71	0.72
1:A:325:ARG:HG2	1:A:325:ARG:HH11	1.54	0.71
1:A:96:VAL:HG23	6:A:2074:HOH:O	1.89	0.71
1:A:297:CYS:SG	4:A:504:G3H:C1	2.80	0.70
1:A:331:ASP:HB2	1:A:334:VAL:HG23	1.72	0.69
1:A:342:PRO:HA	1:A:371:PRO:O	1.92	0.69
1:A:156:GLU:OE2	1:A:486:LYS:HE2	1.92	0.69
1:A:42:LEU:HD23	1:A:42:LEU:O	1.93	0.69
1:A:231:VAL:O	1:A:258:LYS:HE3	1.92	0.69
1:A:143:THR:HG21	6:A:2099:HOH:O	1.92	0.68
1:A:158:LEU:HD21	1:A:484:ALA:HB2	1.75	0.68
1:A:143:THR:HG22	1:A:146:THR:H	1.59	0.68
1:A:155:ARG:HB2	3:A:503:AMP:N1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HB2	1:A:308:PRO:HD3	1.78	0.65
1:A:94:LEU:HD23	1:A:94:LEU:C	2.21	0.65
1:A:155:ARG:HH11	1:A:483:THR:HG22	1.61	0.65
1:A:261:VAL:HG22	1:A:481:ALA:CB	2.28	0.64
1:A:268:ASP:OD2	1:A:424:ASP:HB2	1.98	0.63
1:A:169:TYR:CE1	4:A:504:G3H:H32	2.34	0.63
1:A:95:ASP:O	1:A:99:GLU:HG3	1.98	0.63
1:A:155:ARG:H	3:A:503:AMP:N6	1.97	0.62
1:A:331:ASP:C	1:A:333:THR:H	2.07	0.61
1:A:63:LEU:HD13	1:A:189:VAL:HG22	1.80	0.61
1:A:156:GLU:OE2	6:A:2115:HOH:O	2.16	0.61
1:A:331:ASP:HB3	1:A:333:THR:OG1	2.02	0.60
1:A:169:TYR:CZ	4:A:504:G3H:H32	2.37	0.60
1:A:314:VAL:CG1	1:A:363:LEU:HD13	2.32	0.59
1:A:80:LEU:HD13	1:A:183:ILE:HD11	1.84	0.59
1:A:349:MET:HE1	1:A:366:GLY:O	2.03	0.59
1:A:229:LYS:HG3	6:A:2140:HOH:O	2.03	0.58
1:A:386:VAL:HG23	1:A:389:MET:HE3	1.85	0.58
1:A:320:ARG:O	1:A:324:LEU:HD13	2.04	0.58
1:A:331:ASP:C	1:A:333:THR:N	2.61	0.57
1:A:386:VAL:HG23	1:A:389:MET:CE	2.34	0.57
1:A:479:VAL:O	1:A:483:THR:HB	2.05	0.57
1:A:63:LEU:CD1	1:A:189:VAL:HG22	2.34	0.57
1:A:348:MET:O	1:A:352:ILE:HG13	2.04	0.57
1:A:133:ILE:O	3:A:503:AMP:C6	2.58	0.56
1:A:307:ARG:HB2	1:A:308:PRO:CD	2.34	0.56
1:A:330:ARG:HB2	6:A:2190:HOH:O	2.05	0.56
1:A:381:ALA:HB2	1:A:389:MET:HE1	1.87	0.56
1:A:223:PRO:HG2	1:A:226:GLU:HG3	1.87	0.56
1:A:52:SER:OG	1:A:55:GLU:HG3	2.06	0.56
1:A:367:ARG:HB2	1:A:375:GLN:OE1	2.06	0.56
1:A:352:ILE:O	1:A:356:VAL:HG23	2.06	0.56
1:A:310:TYR:OH	1:A:380:GLU:HG3	2.05	0.55
1:A:407:LYS:HG2	1:A:411:GLN:OE1	2.06	0.55
1:A:470:VAL:HG22	1:A:471:PHE:HD1	1.71	0.55
1:A:345:VAL:HG13	1:A:374:VAL:CG1	2.37	0.54
1:A:342:PRO:HG2	6:A:2197:HOH:O	2.06	0.54
1:A:343:SER:HB2	6:A:2197:HOH:O	2.07	0.54
1:A:325:ARG:HG2	1:A:325:ARG:NH1	2.22	0.53
1:A:398:ALA:HB1	1:A:399:PRO:HD2	1.89	0.53
1:A:307:ARG:HH11	1:A:307:ARG:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HG3	6:A:2094:HOH:O	2.07	0.53
1:A:155:ARG:HH11	1:A:483:THR:CG2	2.22	0.53
1:A:381:ALA:HB1	1:A:389:MET:HE1	1.90	0.53
1:A:243:GLY:HA2	2:A:502:NAP:C5D	2.36	0.52
1:A:470:VAL:O	1:A:471:PHE:HB2	2.09	0.52
1:A:345:VAL:HG13	1:A:374:VAL:HG11	1.92	0.52
1:A:310:TYR:CZ	1:A:314:VAL:HG21	2.44	0.52
1:A:84:ARG:NE	6:A:2061:HOH:O	2.32	0.51
1:A:290:TYR:CD2	1:A:324:LEU:HD21	2.45	0.51
1:A:167:PHE:C	1:A:167:PHE:CD1	2.89	0.51
1:A:220:LEU:HD12	1:A:230:ILE:CD1	2.40	0.51
1:A:331:ASP:O	1:A:333:THR:N	2.45	0.49
1:A:155:ARG:NH1	1:A:483:THR:HG22	2.26	0.48
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.28	0.48
1:A:178:ILE:HD11	1:A:190:VAL:HG21	1.94	0.48
1:A:156:GLU:OE2	1:A:486:LYS:CE	2.60	0.48
1:A:232:ALA:HB2	1:A:254:VAL:CG1	2.44	0.47
1:A:386:VAL:CA	1:A:389:MET:HE2	2.33	0.47
1:A:304:LEU:HD23	1:A:404:VAL:HB	1.97	0.47
1:A:213:PRO:HB2	1:A:216:ALA:HB3	1.97	0.46
1:A:431:ASP:CB	1:A:434:LYS:HE3	2.45	0.46
1:A:322:SER:HA	6:A:2184:HOH:O	2.15	0.46
1:A:431:ASP:HB3	1:A:434:LYS:HE3	1.98	0.46
1:A:141:ASP:HA	1:A:147:LEU:HD12	1.98	0.46
1:A:317:VAL:O	1:A:321:LEU:HG	2.16	0.46
1:A:155:ARG:HB2	3:A:503:AMP:C2	2.51	0.45
1:A:155:ARG:HB2	3:A:503:AMP:C6	2.51	0.45
1:A:339:LEU:HD22	1:A:345:VAL:HG22	1.97	0.45
1:A:19:TYR:O	1:A:48:VAL:HA	2.16	0.45
1:A:6:LEU:HB3	1:A:10:ILE:HG13	1.99	0.45
1:A:314:VAL:HG13	1:A:363:LEU:HD13	1.99	0.45
1:A:327:GLY:O	1:A:373:TYR:HE2	2.00	0.45
1:A:324:LEU:HD23	1:A:376:PRO:HG3	2.00	0.44
1:A:133:ILE:O	3:A:503:AMP:N1	2.50	0.44
1:A:127:GLU:HG2	1:A:128:LEU:N	2.32	0.44
1:A:390:VAL:HG13	1:A:394:ARG:HE	1.82	0.44
1:A:212:PHE:O	1:A:213:PRO:C	2.62	0.43
1:A:386:VAL:HA	1:A:389:MET:CE	2.35	0.43
1:A:387:LYS:NZ	1:A:414:GLU:OE1	2.43	0.43
1:A:391:LEU:HD23	1:A:396:VAL:HG21	1.99	0.43
1:A:301:LYS:HE3	6:A:2222:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:O	1:A:324:LEU:HB2	2.20	0.42
1:A:155:ARG:HB3	1:A:483:THR:CG2	2.48	0.42
1:A:424:ASP:HA	1:A:446:ALA:O	2.18	0.42
1:A:94:LEU:C	1:A:94:LEU:CD2	2.90	0.42
1:A:320:ARG:HH11	1:A:320:ARG:HG3	1.85	0.42
1:A:445:GLY:HA3	1:A:463:GLY:O	2.20	0.42
1:A:476:GLY:O	1:A:479:VAL:HG12	2.20	0.42
1:A:233:ASP:OD1	1:A:235:ARG:CD	2.61	0.42
1:A:263:GLU:HB3	6:A:2164:HOH:O	2.19	0.42
1:A:104:ASN:O	1:A:104:ASN:ND2	2.53	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.88	0.41
1:A:297:CYS:SG	1:A:298:ASP:N	2.93	0.41
1:A:201:ALA:HA	1:A:219:LEU:CD2	2.51	0.41
1:A:266:GLY:O	1:A:297:CYS:O	2.39	0.41
1:A:102:VAL:HG13	1:A:329:PRO:HB2	2.02	0.41
1:A:283:ASP:O	1:A:287:ARG:HG3	2.22	0.40
1:A:143:THR:HG22	1:A:146:THR:N	2.32	0.40
1:A:431:ASP:CG	1:A:434:LYS:HE3	2.46	0.40
1:A:327:GLY:O	1:A:373:TYR:CE2	2.74	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	497/501 (99%)	468 (94%)	26 (5%)	3 (1%)	21 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	GLY
1	A	7	GLU

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Mol	Chain	Res	Type
1	A	42	LEU

5.3.2 Protein sidechains ⓘ

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	386/393 (98%)	364 (94%)	22 (6%)	18	19

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

Mol	Chain	Res	Type
1	A	26	GLU
1	A	42	LEU
1	A	80	LEU
1	A	92	ARG
1	A	96	VAL
1	A	127	GLU
1	A	133	ILE
1	A	143	THR
1	A	147	LEU
1	A	149	THR
1	A	152	LEU
1	A	165	THR
1	A	166	PRO
1	A	191	LYS
1	A	194	ILE
1	A	235	ARG
1	A	261	VAL
1	A	301	LYS
1	A	324	LEU
1	A	424	ASP
1	A	472	ARG
1	A	483	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
3	AMP	A	503	-	25,25,25	1.89	7 (28%)	37,38,38	1.68	10 (27%)
4	G3H	A	504	-	8,9,9	0.87	0	7,12,12	0.87	0
2	NAP	A	502	-	42,42,52	1.44	6 (14%)	60,65,80	1.78	10 (16%)

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	AMP	A	503	-	-	1/10/26/26	0/3/3/3
4	G3H	A	504	-	-	6/7/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	502	-	-	14/27/56/67	0/4/4/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	AMP	C3'-C4'	5.64	1.67	1.53
2	A	502	NAP	P2B-O2B	3.60	1.65	1.59
2	A	502	NAP	C5A-N7A	-3.51	1.32	1.39
2	A	502	NAP	PN-O3	-3.18	1.56	1.59
3	A	503	AMP	O3'-C3'	2.76	1.49	1.43
3	A	503	AMP	C2'-C1'	2.28	1.60	1.53
3	A	503	AMP	C6-N1	2.26	1.42	1.35
3	A	503	AMP	C2'-C3'	2.22	1.59	1.53
2	A	502	NAP	C4A-N3A	2.20	1.38	1.34
2	A	502	NAP	C4A-N9A	-2.18	1.33	1.37
3	A	503	AMP	P-O2P	-2.16	1.46	1.54
2	A	502	NAP	C8A-N7A	2.12	1.35	1.31
3	A	503	AMP	C5-C4	2.10	1.42	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAP	C5A-C4A-N3A	-5.77	118.77	126.72
2	A	502	NAP	N3A-C2A-N1A	-5.14	120.80	128.58
2	A	502	NAP	N3A-C4A-N9A	4.76	135.27	127.17
2	A	502	NAP	O4B-C4B-C5B	-4.60	94.61	109.33
2	A	502	NAP	C2A-N3A-C4A	3.81	121.14	111.83
3	A	503	AMP	N6-C6-N1	3.38	125.91	118.38
3	A	503	AMP	O4'-C4'-C5'	-3.33	98.66	109.33
3	A	503	AMP	C4-C5-N7	3.09	114.11	110.58
3	A	503	AMP	C5-N7-C8	-3.03	98.69	103.45
3	A	503	AMP	N3-C2-N1	-2.69	124.50	128.58
3	A	503	AMP	C2-N1-C6	2.56	122.94	118.73
2	A	502	NAP	N9A-C8A-N7A	-2.52	110.36	113.94
2	A	502	NAP	C6A-C5A-C4A	2.43	120.50	117.18
2	A	502	NAP	C6A-C5A-N7A	-2.34	127.58	132.09
3	A	503	AMP	N9-C8-N7	2.33	117.23	113.94
3	A	503	AMP	O2P-P-O1P	2.23	119.53	110.83
2	A	502	NAP	O4B-C1B-C2B	-2.13	102.92	106.59
3	A	503	AMP	C5-C6-N6	-2.13	118.02	123.29
3	A	503	AMP	O3'-C3'-C4'	-2.12	104.98	111.08
2	A	502	NAP	C5B-C4B-C3B	-2.00	108.00	115.21

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	NAP	PN-O3-PA-O5B
2	A	502	NAP	C5D-O5D-PN-O1N
2	A	502	NAP	C5D-O5D-PN-O2N
4	A	504	G3H	O1-C1-C2-C3
4	A	504	G3H	C1-C2-C3-O1P
4	A	504	G3H	O2-C2-C3-O1P
4	A	504	G3H	C3-O1P-P-O2P
4	A	504	G3H	C3-O1P-P-O3P
4	A	504	G3H	C3-O1P-P-O4P
2	A	502	NAP	O4D-C4D-C5D-O5D
2	A	502	NAP	C3D-C4D-C5D-O5D
2	A	502	NAP	C2B-C1B-N9A-C8A
2	A	502	NAP	C4D-C5D-O5D-PN
2	A	502	NAP	C5D-O5D-PN-O3
2	A	502	NAP	PA-O3-PN-O2N
2	A	502	NAP	C2B-C1B-N9A-C4A
2	A	502	NAP	C2B-O2B-P2B-O2X
3	A	503	AMP	C2'-C1'-N9-C8
2	A	502	NAP	O4B-C1B-N9A-C8A
2	A	502	NAP	PA-O3-PN-O1N
2	A	502	NAP	O4B-C4B-C5B-O5B

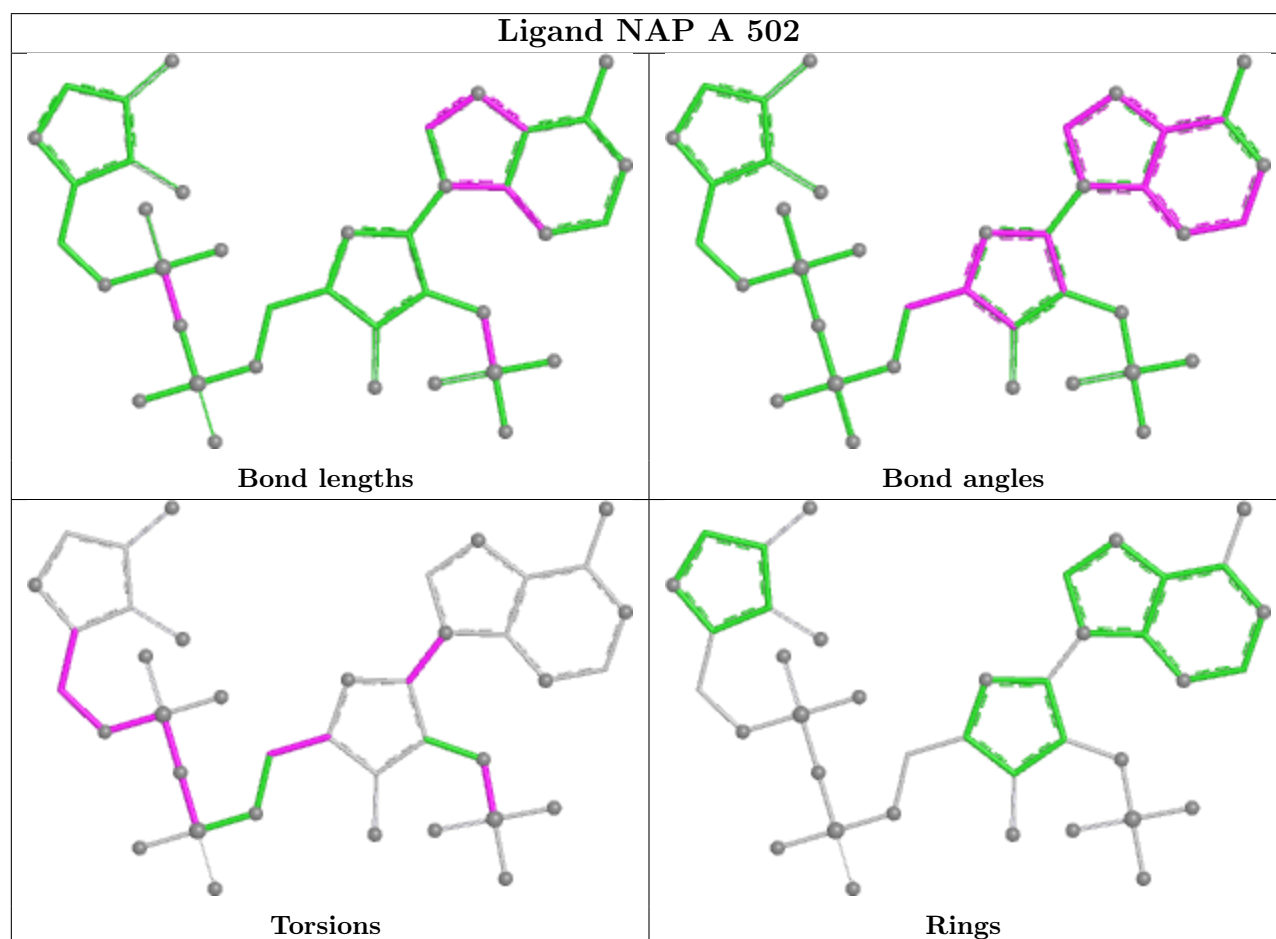
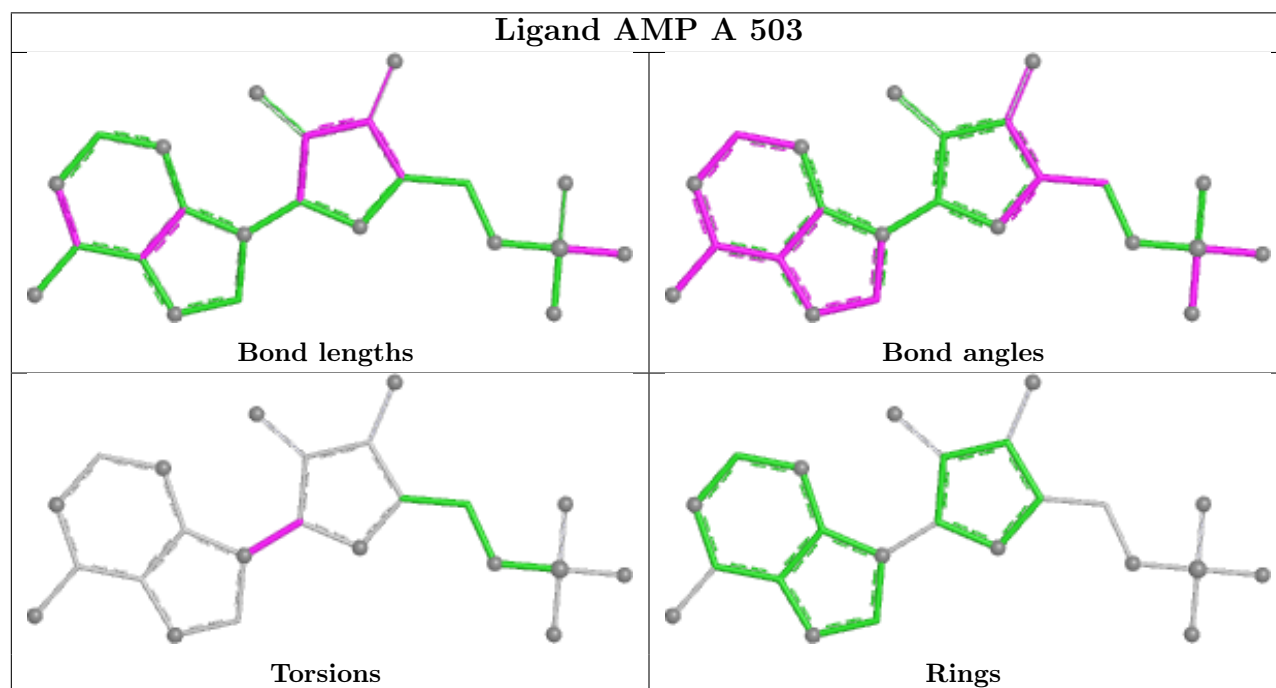
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	AMP	6	0
4	A	504	G3H	3	0
2	A	502	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	499/501 (99%)	0.92	64 (12%) 7 7	32, 49, 74, 91	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	TYR	7.3
1	A	334	VAL	6.3
1	A	3	ALA	5.8
1	A	327	GLY	5.6
1	A	328	ASP	5.6
1	A	333	THR	5.0
1	A	134	GLY	4.2
1	A	332	PRO	4.0
1	A	326	VAL	4.0
1	A	329	PRO	3.8
1	A	137	TYR	3.6
1	A	331	ASP	3.6
1	A	4	GLY	3.5
1	A	373	TYR	3.4
1	A	336	VAL	3.2
1	A	10	ILE	3.2
1	A	13	LYS	3.0
1	A	127	GLU	3.0
1	A	324	LEU	3.0
1	A	14	GLY	3.0
1	A	42	LEU	3.0
1	A	323	SER	3.0
1	A	54	GLU	3.0
1	A	99	GLU	3.0
1	A	360	GLY	2.9
1	A	325	ARG	2.9
1	A	109	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	322	SER	2.7
1	A	330	ARG	2.7
1	A	381	ALA	2.7
1	A	362	VAL	2.7
1	A	394	ARG	2.7
1	A	407	LYS	2.6
1	A	5	LEU	2.6
1	A	66	ARG	2.5
1	A	12	GLU	2.5
1	A	316	GLU	2.5
1	A	144	TYR	2.5
1	A	145	ASP	2.5
1	A	267	GLY	2.4
1	A	133	ILE	2.4
1	A	195	SER	2.3
1	A	353	GLU	2.3
1	A	307	ARG	2.3
1	A	343	SER	2.3
1	A	471	PHE	2.2
1	A	246	GLU	2.2
1	A	9	VAL	2.2
1	A	40	ILE	2.2
1	A	345	VAL	2.2
1	A	357	GLU	2.2
1	A	29	GLY	2.2
1	A	11	LYS	2.1
1	A	26	GLU	2.1
1	A	129	ASP	2.1
1	A	501	GLU	2.1
1	A	374	VAL	2.1
1	A	337	GLY	2.1
1	A	226	GLU	2.0
1	A	58	ARG	2.0
1	A	7	GLU	2.0
1	A	110	SER	2.0
1	A	367	ARG	2.0
1	A	312	LYS	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](#)

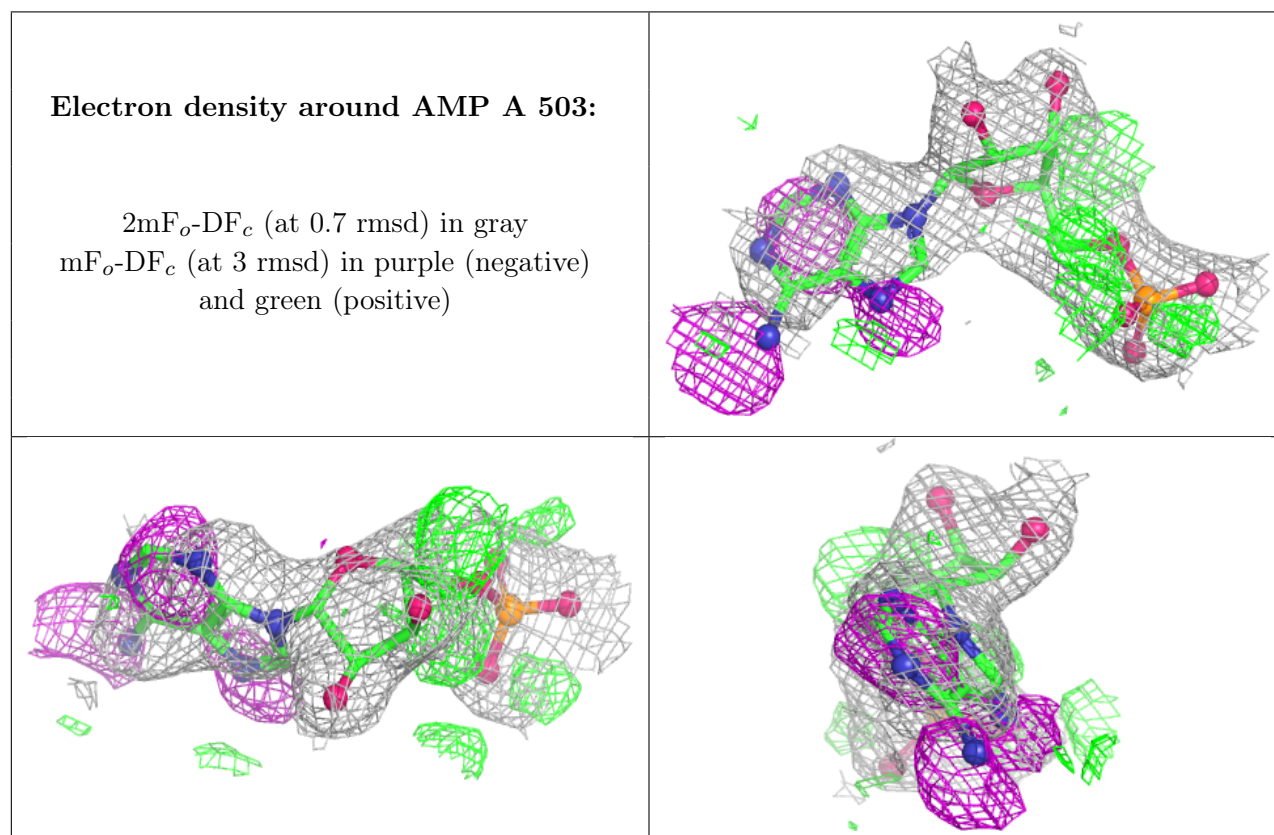
There are no oligosaccharides in this entry.

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.

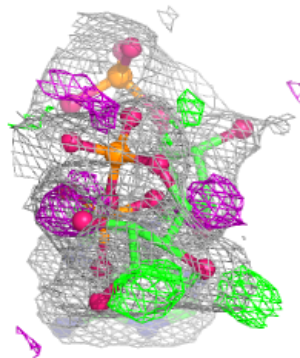
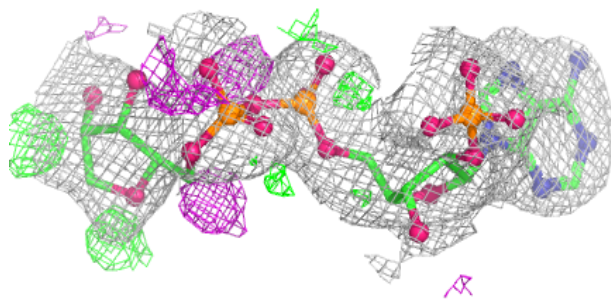
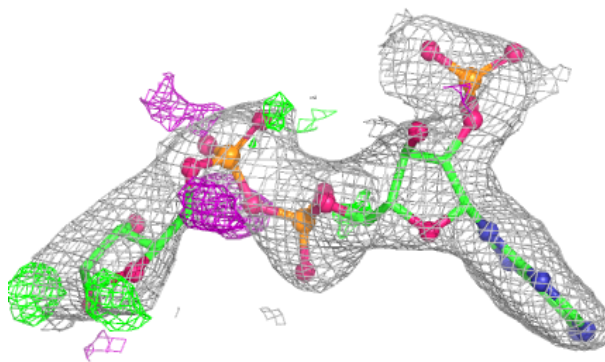
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	A	503	23/23	0.91	0.19	44,51,72,75	0
2	NAP	A	502	39/48	0.92	0.13	51,62,79,82	0
4	G3H	A	504	10/10	0.93	0.13	47,50,53,54	0
5	NA	A	754	1/1	0.99	0.05	46,46,46,46	0

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 NAP A 502:

$2mF_o-DF_c$ (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.