



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 8JB1 / pdb_00008jb1
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from
Corynebacterium glutamicum ATCC13032 in complex with NADP
Authors : Son, H.F.; Kim, K.J.
Deposited on : 2023-05-07
Resolution : 2.44 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

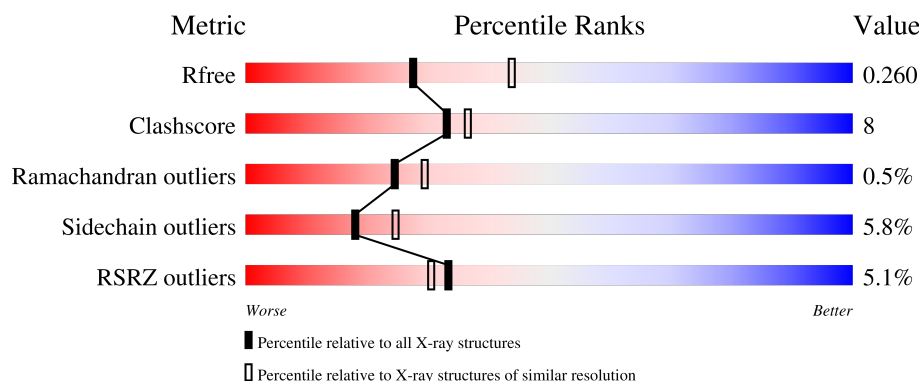
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

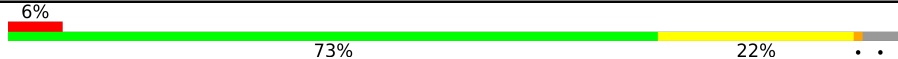
The reported resolution of this entry is 2.44 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	488	
1	B	488	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7536 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.

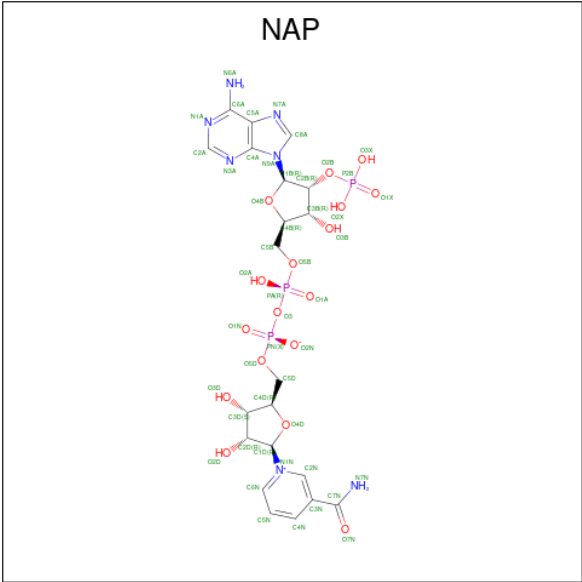
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3651	2288	657	701	5			
1	B	468	Total	C	N	O	S	0	0	0
			3641	2282	653	701	5			

There are 16 discrepancies between the modelled and reference sequences:

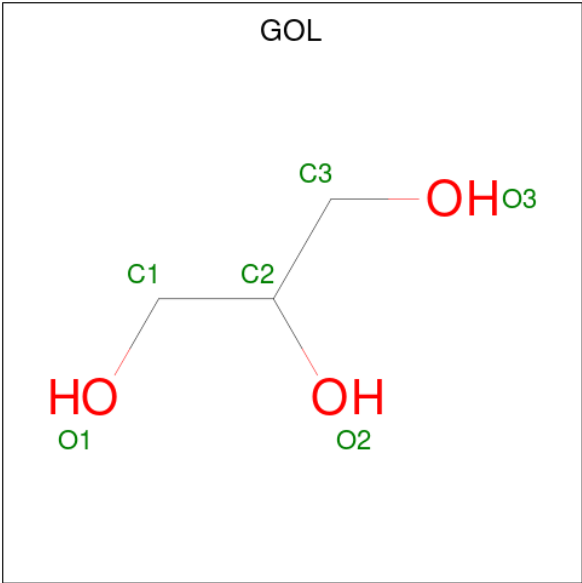
Chain	Residue	Modelled	Actual	Comment	Reference
A	481	LEU	-	expression tag	UNP A0A8G0FZM1
A	482	GLU	-	expression tag	UNP A0A8G0FZM1
A	483	HIS	-	expression tag	UNP A0A8G0FZM1
A	484	HIS	-	expression tag	UNP A0A8G0FZM1
A	485	HIS	-	expression tag	UNP A0A8G0FZM1
A	486	HIS	-	expression tag	UNP A0A8G0FZM1
A	487	HIS	-	expression tag	UNP A0A8G0FZM1
A	488	HIS	-	expression tag	UNP A0A8G0FZM1
B	481	LEU	-	expression tag	UNP A0A8G0FZM1
B	482	GLU	-	expression tag	UNP A0A8G0FZM1
B	483	HIS	-	expression tag	UNP A0A8G0FZM1
B	484	HIS	-	expression tag	UNP A0A8G0FZM1
B	485	HIS	-	expression tag	UNP A0A8G0FZM1
B	486	HIS	-	expression tag	UNP A0A8G0FZM1
B	487	HIS	-	expression tag	UNP A0A8G0FZM1
B	488	HIS	-	expression tag	UNP A0A8G0FZM1

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

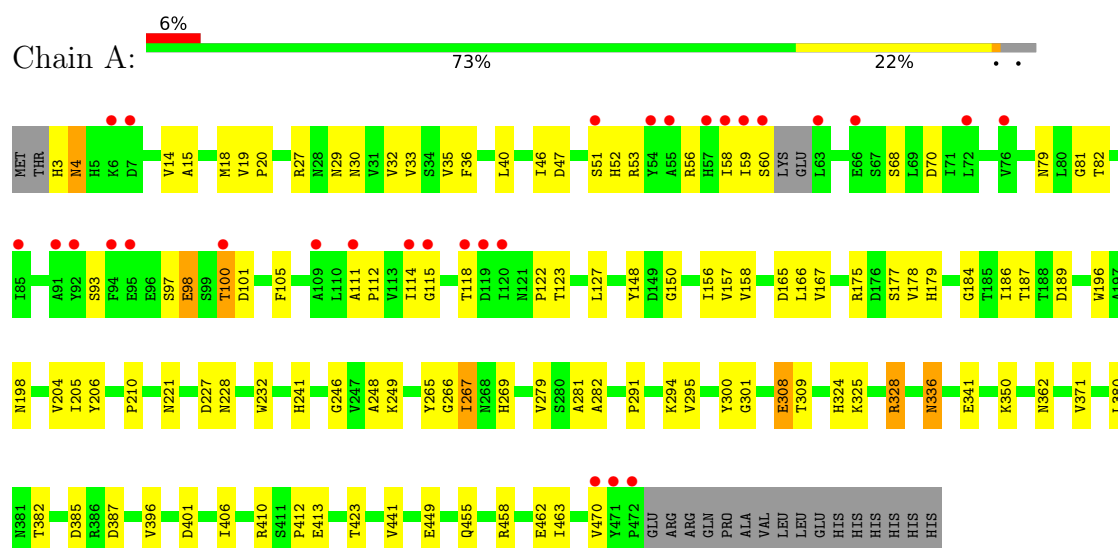
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	73	Total	O	0	0
			73	73		

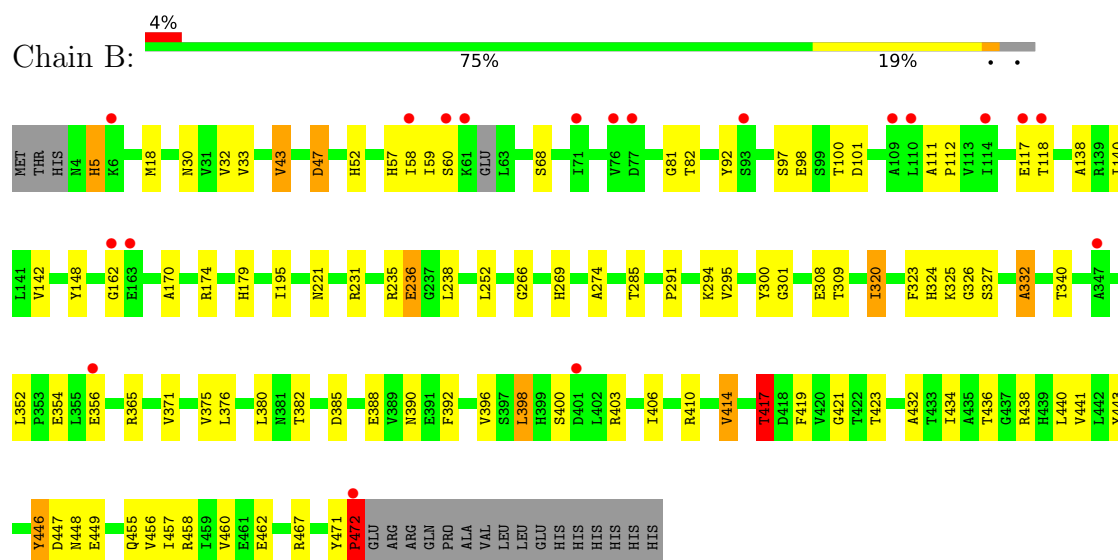
3 Residue-property plots [i](#)

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: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.75Å 92.75Å 287.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.54 – 2.44 31.54 – 2.44	Depositor EDS
% Data completeness (in resolution range)	94.8 (31.54-2.44) 94.8 (31.54-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.192 , 0.262 0.197 , 0.260	Depositor DCC
R_{free} test set	2189 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0123e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, NAP

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	0.64	0/3712	1.18	11/5047 (0.2%)
1	B	0.65	0/3701	1.15	13/5032 (0.3%)
All	All	0.64	0/7413	1.17	24/10079 (0.2%)

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	A	0	2
1	B	0	6
All	All	0	8

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	TYR	CA-C-N	-9.72	115.47	122.18
1	A	300	TYR	C-N-CA	-9.72	115.47	122.18
1	B	5	HIS	CA-CB-CG	7.27	121.07	113.80
1	A	308	GLU	CB-CG-CD	7.00	124.50	112.60
1	A	387	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	309	THR	CA-CB-OG1	-6.46	99.92	109.60
1	B	423	THR	CB-CA-C	6.31	120.63	110.09
1	A	336	ASN	CA-C-N	5.69	129.64	121.50
1	A	336	ASN	C-N-CA	5.69	129.64	121.50
1	A	70	ASP	CB-CA-C	5.62	119.77	110.90
1	B	320	ILE	CB-CA-C	5.61	120.75	110.71
1	A	309	THR	CA-CB-OG1	-5.47	101.39	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	VAL	CB-CA-C	-5.44	105.38	111.80
1	B	417	THR	CA-CB-OG1	-5.39	101.51	109.60
1	B	462	GLU	CB-CA-C	-5.18	102.53	110.81
1	B	308	GLU	CB-CA-C	-5.12	101.79	110.19
1	B	472	PRO	N-CA-CB	-5.12	97.37	103.00
1	B	332	ALA	CA-C-N	5.11	127.63	120.28
1	B	332	ALA	C-N-CA	5.11	127.63	120.28
1	B	308	GLU	CA-C-N	-5.09	115.98	123.00
1	B	308	GLU	C-N-CA	-5.09	115.98	123.00
1	A	189	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	228	ASN	CB-CA-C	5.05	119.20	111.02
1	B	47	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASN	Peptide
1	A	410	ARG	Sidechain
1	B	162	GLY	Peptide
1	B	174	ARG	Sidechain
1	B	231	ARG	Sidechain
1	B	365	ARG	Sidechain
1	B	410	ARG	Sidechain
1	B	467	ARG	Sidechain

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	3651	0	3642	57	0
1	B	3641	0	3628	62	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
3	A	6	0	8	1	0
3	B	12	0	16	5	0
4	A	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	73	0	0	1	0
All	All	7536	0	7344	115	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 8.

All (115) 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:291:PRO:HB2	1:A:406:ILE:HD11	1.24	1.10
1:B:179:HIS:HD2	3:B:502:GOL:O2	1.49	0.95
1:B:179:HIS:CD2	3:B:502:GOL:O2	2.20	0.95
1:B:30:ASN:HB2	1:B:82:THR:HG22	1.60	0.82
1:A:291:PRO:CB	1:A:406:ILE:HD11	2.11	0.77
1:B:179:HIS:HE1	1:B:449:GLU:OE1	1.68	0.75
1:A:81:GLY:HA2	1:A:118:THR:HG22	1.69	0.73
1:B:179:HIS:HD2	3:B:502:GOL:HO2	1.35	0.73
1:B:81:GLY:HA2	1:B:118:THR:HG22	1.70	0.73
1:A:266:GLY:H	1:A:269:HIS:CD2	2.10	0.69
1:A:210:PRO:HG3	1:A:232:TRP:CH2	2.29	0.67
1:B:82:THR:HG23	1:B:118:THR:HA	1.77	0.67
1:A:265:TYR:HE2	1:A:462:GLU:HG3	1.59	0.67
1:B:97:SER:HB3	1:B:98:GLU:HA	1.77	0.66
1:B:43:VAL:HG13	1:B:47:ASP:HB2	1.79	0.64
1:A:266:GLY:H	1:A:269:HIS:HD2	1.45	0.64
1:A:29:ASN:O	1:A:81:GLY:O	2.16	0.62
1:A:47:ASP:O	1:A:51:SER:HB2	1.99	0.61
1:B:57:HIS:O	1:B:398:LEU:CD1	2.49	0.60
1:A:301:GLY:O	1:A:380:LEU:HA	2.01	0.60
1:B:170:ALA:HB2	1:B:195:ILE:HD12	1.84	0.59
1:A:59:ILE:O	1:A:60:SER:HB2	2.03	0.59
1:A:265:TYR:CE2	1:A:462:GLU:HG3	2.38	0.59
1:B:140:ILE:HG21	1:B:457:ILE:HG13	1.86	0.58
1:B:285:THR:OG1	3:B:503:GOL:H12	2.03	0.58
1:A:32:VAL:HG21	1:A:148:TYR:CE1	2.39	0.58
1:B:434:ILE:O	1:B:440:LEU:HD12	2.03	0.58
1:B:455:GLN:OE1	1:B:458:ARG:NH1	2.37	0.58
1:A:328:ARG:HH21	1:A:328:ARG:HB2	1.68	0.58
1:B:324:HIS:CD2	1:B:326:GLY:H	2.23	0.57
1:A:187:THR:OG1	1:B:5:HIS:HE1	1.89	0.56
1:B:392:PHE:O	1:B:396:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:THR:HB	1:B:101:ASP:HA	1.88	0.55
1:B:320:ILE:HA	1:B:332:ALA:HB2	1.90	0.54
1:B:421:GLY:HA3	3:B:502:GOL:H32	1.91	0.53
1:B:446:TYR:N	1:B:446:TYR:CD1	2.76	0.53
1:A:15:ALA:O	1:A:18:MET:HB2	2.08	0.53
1:A:184:GLY:HA3	1:A:198:ASN:OD1	2.09	0.52
1:B:448:ASN:HD22	2:B:501:NAP:H72N	1.56	0.52
1:B:438:ARG:HD3	4:B:673:HOH:O	2.08	0.52
1:A:187:THR:OG1	1:B:5:HIS:CE1	2.62	0.52
1:A:179:HIS:HE1	1:A:449:GLU:OE1	1.90	0.52
1:A:455:GLN:OE1	1:A:458:ARG:NH1	2.43	0.51
1:B:324:HIS:HD2	1:B:326:GLY:H	1.56	0.51
1:B:179:HIS:CE1	1:B:449:GLU:OE1	2.58	0.51
1:B:414:VAL:CG1	1:B:419:PHE:CE2	2.95	0.50
1:B:456:VAL:O	1:B:460:VAL:HG23	2.11	0.50
1:A:52:HIS:HE1	1:A:68:SER:OG	1.94	0.50
1:B:300:TYR:OH	1:B:388:GLU:OE1	2.23	0.50
1:A:157:VAL:HA	1:A:205:ILE:O	2.12	0.50
1:A:98:GLU:H	1:A:98:GLU:CD	2.20	0.49
1:A:177:SER:HA	1:B:417:THR:HG21	1.92	0.49
1:B:18:MET:HE3	1:B:68:SER:HB3	1.93	0.49
1:A:227:ASP:OD2	1:A:241:HIS:HE1	1.95	0.48
1:B:291:PRO:CB	1:B:406:ILE:HD11	2.44	0.48
1:A:175:ARG:HG2	1:A:175:ARG:HH21	1.78	0.48
1:A:166:LEU:HD12	1:A:204:VAL:HG21	1.95	0.48
1:A:111:ALA:N	1:A:112:PRO:CD	2.77	0.48
1:A:122:PRO:HA	1:A:150:GLY:O	2.14	0.48
1:A:221:ASN:HD22	1:A:246:GLY:HA2	1.79	0.47
1:A:52:HIS:CE1	1:A:68:SER:OG	2.68	0.47
1:B:323:PHE:CD1	1:B:324:HIS:N	2.82	0.47
1:B:414:VAL:HG11	1:B:419:PHE:CZ	2.50	0.47
1:A:93:SER:O	1:A:105:PHE:CZ	2.68	0.47
1:A:281:ALA:O	1:A:282:ALA:HB3	2.15	0.47
1:B:375:VAL:HG22	1:B:443:TYR:CD2	2.49	0.46
1:B:266:GLY:H	1:B:269:HIS:CD2	2.33	0.46
1:B:294:LYS:HB2	1:B:352:LEU:HD11	1.98	0.46
1:A:324:HIS:CD2	1:A:325:LYS:H	2.34	0.45
1:B:376:LEU:O	1:B:441:VAL:HA	2.17	0.45
1:B:414:VAL:CG1	1:B:419:PHE:CZ	2.99	0.45
1:A:36:PHE:CB	1:A:58:ILE:HD13	2.47	0.45
1:B:396:VAL:HA	1:B:400:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PHE:HB3	1:A:58:ILE:HD13	1.99	0.44
1:B:301:GLY:O	1:B:380:LEU:HA	2.17	0.44
1:A:35:VAL:HG23	1:A:40:LEU:HD11	1.99	0.43
1:B:59:ILE:HG23	1:B:60:SER:N	2.33	0.43
1:A:14:VAL:O	1:A:15:ALA:C	2.61	0.43
1:A:19:VAL:N	1:A:20:PRO:HD2	2.34	0.43
1:B:238:LEU:HD11	1:B:252:LEU:HD22	2.00	0.43
1:A:198:ASN:O	1:B:5:HIS:HD2	2.01	0.43
1:A:59:ILE:O	1:A:60:SER:CB	2.66	0.43
1:A:186:ILE:HA	1:A:196:TRP:O	2.19	0.43
1:B:432:ALA:HB1	1:B:443:TYR:CD1	2.54	0.43
1:A:100:THR:HA	1:A:101:ASP:C	2.44	0.43
1:A:324:HIS:CD2	1:A:325:LYS:N	2.87	0.42
1:B:447:ASP:OD1	1:B:447:ASP:C	2.61	0.42
1:A:158:VAL:O	1:A:206:TYR:HA	2.18	0.42
1:A:248:ALA:C	1:A:249:LYS:HG3	2.44	0.42
1:B:59:ILE:HD11	1:B:92:TYR:CD1	2.54	0.42
1:B:100:THR:CB	1:B:101:ASP:HA	2.49	0.42
1:A:53:ARG:NH1	1:A:56:ARG:HH11	2.16	0.42
1:B:57:HIS:O	1:B:398:LEU:HD13	2.20	0.42
1:B:82:THR:HG23	1:B:118:THR:CA	2.48	0.42
1:A:265:TYR:HE2	1:A:462:GLU:CG	2.28	0.42
1:A:267:ILE:HD11	1:A:291:PRO:HA	2.01	0.42
1:A:308:GLU:OE2	1:A:362:ASN:HB2	2.20	0.42
1:A:412:PRO:O	1:A:413:GLU:HB2	2.19	0.42
1:B:97:SER:CB	1:B:98:GLU:HA	2.41	0.41
1:A:79:ASN:O	1:A:115:GLY:N	2.53	0.41
1:B:111:ALA:N	1:B:112:PRO:CD	2.83	0.41
1:B:291:PRO:HB2	1:B:406:ILE:HD11	2.03	0.41
1:B:471:TYR:HA	1:B:472:PRO:HA	1.86	0.41
1:A:4:ASN:C	1:A:4:ASN:HD22	2.29	0.41
1:B:138:ALA:O	1:B:142:VAL:HG23	2.21	0.41
1:A:127:LEU:O	1:A:156:ILE:HA	2.21	0.41
1:B:400:SER:O	1:B:403:ARG:HB2	2.21	0.41
1:B:446:TYR:N	1:B:446:TYR:HD1	2.18	0.41
1:B:32:VAL:HG21	1:B:148:TYR:CE1	2.55	0.41
1:B:235:ARG:O	1:B:236:GLU:C	2.64	0.40
1:A:27:ARG:HH11	1:A:27:ARG:HG2	1.86	0.40
1:B:52:HIS:HE1	1:B:68:SER:OG	2.03	0.40
1:B:266:GLY:H	1:B:269:HIS:HD2	1.70	0.40
1:A:30:ASN:HD22	1:A:118:THR:HB	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:HD2	3:A:502:GOL:O1	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	464/488 (95%)	440 (95%)	22 (5%)	2 (0%)	30	36
1	B	464/488 (95%)	428 (92%)	33 (7%)	3 (1%)	21	25
All	All	928/976 (95%)	868 (94%)	55 (6%)	5 (0%)	24	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	SER
1	A	114	ILE
1	B	274	ALA
1	B	371	VAL
1	A	371	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/417 (95%)	372 (94%)	26 (6%)	15	20
1	B	396/417 (95%)	376 (95%)	20 (5%)	21	29
All	All	794/834 (95%)	748 (94%)	46 (6%)	18	25

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	ASN
1	A	33	VAL
1	A	46	ILE
1	A	82	THR
1	A	97	SER
1	A	98	GLU
1	A	100	THR
1	A	123	THR
1	A	165	ASP
1	A	167	VAL
1	A	267	ILE
1	A	279	VAL
1	A	294	LYS
1	A	295	VAL
1	A	328	ARG
1	A	341	GLU
1	A	350	LYS
1	A	382	THR
1	A	385	ASP
1	A	396	VAL
1	A	401	ASP
1	A	423	THR
1	A	441	VAL
1	A	463	ILE
1	A	470	VAL
1	B	33	VAL
1	B	43	VAL
1	B	58	ILE
1	B	117	GLU
1	B	221	ASN
1	B	236	GLU

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Mol	Chain	Res	Type
1	B	295	VAL
1	B	325	LYS
1	B	340	THR
1	B	354	GLU
1	B	356	GLU
1	B	382	THR
1	B	385	ASP
1	B	390	ASN
1	B	398	LEU
1	B	414	VAL
1	B	417	THR
1	B	436	THR
1	B	446	TYR
1	B	472	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	HIS
1	A	29	ASN
1	A	30	ASN
1	A	52	HIS
1	A	89	GLN
1	A	179	HIS
1	A	192	ASN
1	A	221	ASN
1	A	228	ASN
1	A	240	GLN
1	A	241	HIS
1	A	269	HIS
1	A	324	HIS
1	A	381	ASN
1	A	390	ASN
1	A	454	ASN
1	B	4	ASN
1	B	5	HIS
1	B	29	ASN
1	B	52	HIS
1	B	79	ASN
1	B	89	GLN
1	B	179	HIS

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Mol	Chain	Res	Type
1	B	221	ASN
1	B	269	HIS
1	B	297	ASN
1	B	315	ASN
1	B	324	HIS
1	B	390	ASN
1	B	399	HIS
1	B	454	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 ⓘ

5 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	GOL	B	502	-	5,5,5	0.29	0	5,5,5	0.66	0
2	NAP	B	501	-	50,52,52	0.70	2 (4%)	71,80,80	0.93	4 (5%)
3	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.56	0
2	NAP	A	501	-	50,52,52	0.69	0	71,80,80	1.02	7 (9%)
3	GOL	B	503	-	5,5,5	0.19	0	5,5,5	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	502	-	-	4/4/4/4	-
2	NAP	B	501	-	-	6/35/67/67	0/5/5/5
3	GOL	A	502	-	-	4/4/4/4	-
2	NAP	A	501	-	-	6/35/67/67	0/5/5/5
3	GOL	B	503	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAP	O4D-C1D	2.31	1.43	1.40
2	B	501	NAP	C2N-N1N	2.03	1.37	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAP	P2B-O2B-C2B	-3.10	115.14	123.43
2	A	501	NAP	O2A-PA-O1A	3.02	126.50	112.44
2	A	501	NAP	O2B-C2B-C3B	2.55	120.84	111.68
2	B	501	NAP	O3B-C3B-C2B	2.55	118.33	111.19
2	B	501	NAP	O2A-PA-O1A	2.55	124.30	112.44
2	B	501	NAP	C6N-N1N-C2N	-2.37	119.86	121.88
2	A	501	NAP	C2N-C3N-C4N	2.34	120.98	118.26
2	A	501	NAP	O3B-C3B-C4B	-2.24	104.64	111.08
2	A	501	NAP	O2A-PA-O3	-2.14	101.50	107.27
2	A	501	NAP	O4B-C1B-N9A	2.02	111.98	108.09
2	B	501	NAP	O3-PA-O1A	-2.01	104.67	110.70

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	O4D-C1D-N1N-C2N
2	A	501	NAP	O4D-C1D-N1N-C6N
2	A	501	NAP	C2D-C1D-N1N-C2N
2	A	501	NAP	C2D-C1D-N1N-C6N
2	B	501	NAP	O4D-C1D-N1N-C2N

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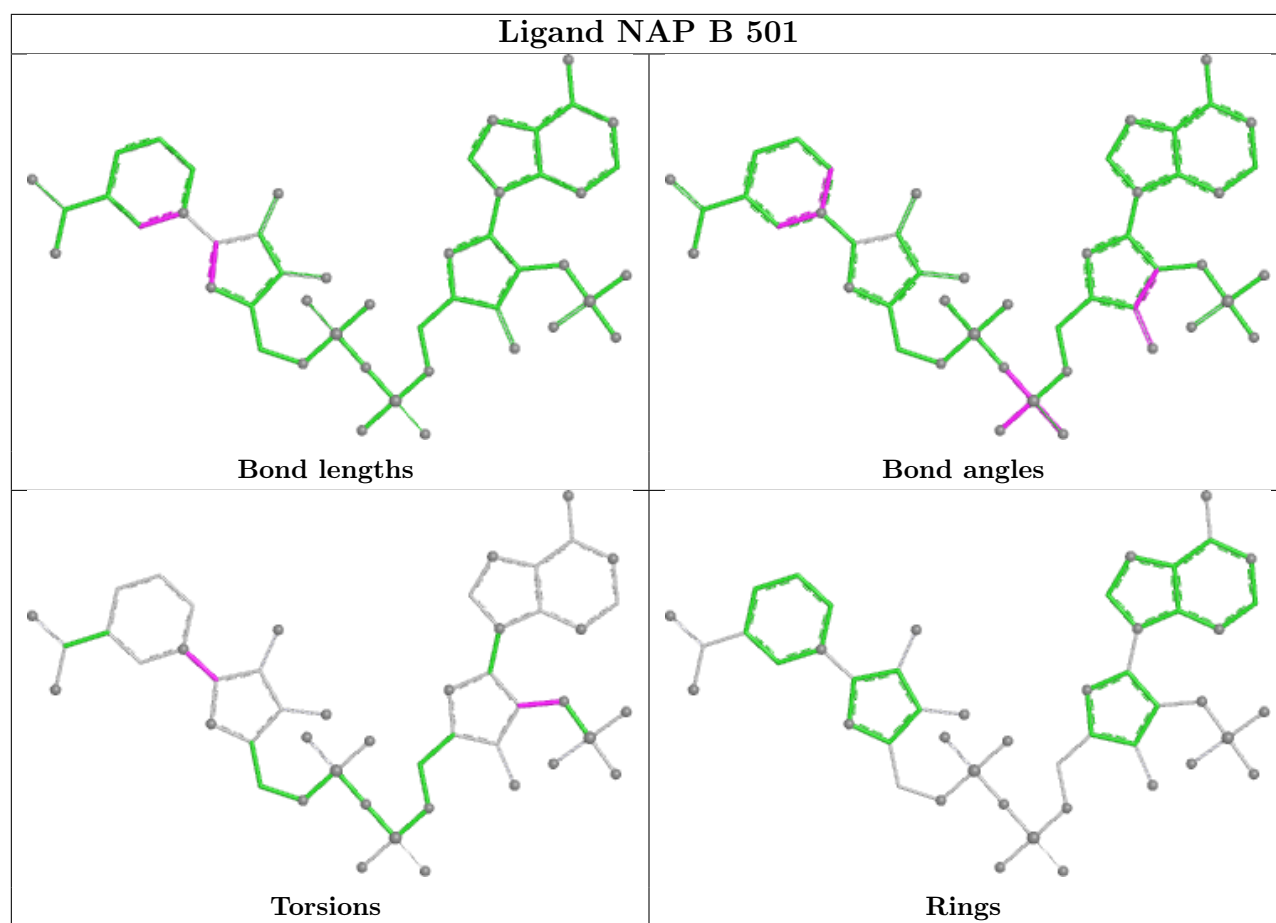
Mol	Chain	Res	Type	Atoms
2	B	501	NAP	O4D-C1D-N1N-C6N
2	B	501	NAP	C2D-C1D-N1N-C6N
3	A	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	C1-C2-C3-O3
3	B	503	GOL	O1-C1-C2-C3
3	B	503	GOL	C1-C2-C3-O3
2	A	501	NAP	C3B-C2B-O2B-P2B
2	B	501	NAP	C3B-C2B-O2B-P2B
3	A	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O2-C2-C3-O3
2	B	501	NAP	C1B-C2B-O2B-P2B
3	A	502	GOL	O2-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
2	B	501	NAP	C2D-C1D-N1N-C2N
3	A	502	GOL	O1-C1-C2-O2
2	A	501	NAP	O4B-C4B-C5B-O5B

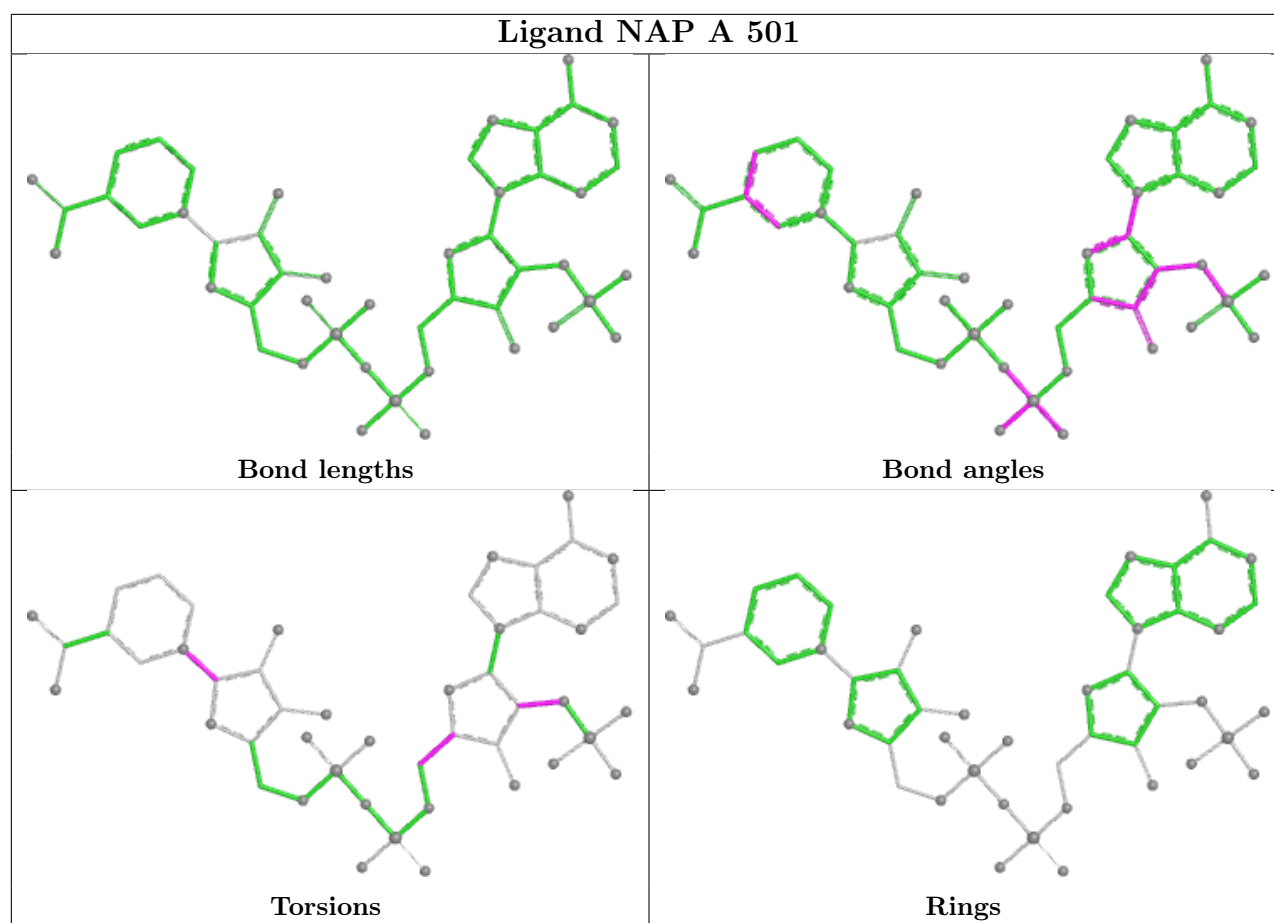
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	GOL	4	0
2	B	501	NAP	1	0
3	A	502	GOL	1	0
3	B	503	GOL	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 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	468/488 (95%)	0.06	29 (6%) 26 23	15, 35, 100, 125	0
1	B	468/488 (95%)	0.01	19 (4%) 41 39	15, 37, 94, 139	0
All	All	936/976 (95%)	0.03	48 (5%) 33 30	15, 36, 98, 139	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ALA	4.4
1	A	76	VAL	3.9
1	B	60	SER	3.9
1	A	114	ILE	3.8
1	B	58	ILE	3.7
1	A	118	THR	3.6
1	A	109	ALA	3.5
1	A	54	TYR	3.4
1	B	109	ALA	3.4
1	A	471	TYR	3.4
1	A	472	PRO	3.4
1	B	61	LYS	3.2
1	B	71	ILE	3.2
1	A	51	SER	3.1
1	B	472	PRO	3.1
1	B	118	THR	3.1
1	B	162	GLY	3.0
1	B	76	VAL	3.0
1	A	58	ILE	3.0
1	B	114	ILE	2.8
1	B	77	ASP	2.7
1	A	92	TYR	2.7
1	A	100	THR	2.7
1	B	110	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	6	LYS	2.5
1	A	55	ALA	2.5
1	A	111	ALA	2.5
1	A	63	LEU	2.4
1	A	66	GLU	2.4
1	A	94	PHE	2.4
1	B	6	LYS	2.4
1	B	347	ALA	2.4
1	B	163	GLU	2.3
1	A	57	HIS	2.3
1	B	401	ASP	2.3
1	A	470	VAL	2.3
1	A	115	GLY	2.3
1	A	120	ILE	2.3
1	A	7	ASP	2.2
1	B	117	GLU	2.2
1	B	356	GLU	2.2
1	A	60	SER	2.2
1	A	72	LEU	2.1
1	A	85	ILE	2.1
1	A	95	GLU	2.1
1	B	93	SER	2.1
1	A	59	ILE	2.0
1	A	119	ASP	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](#)

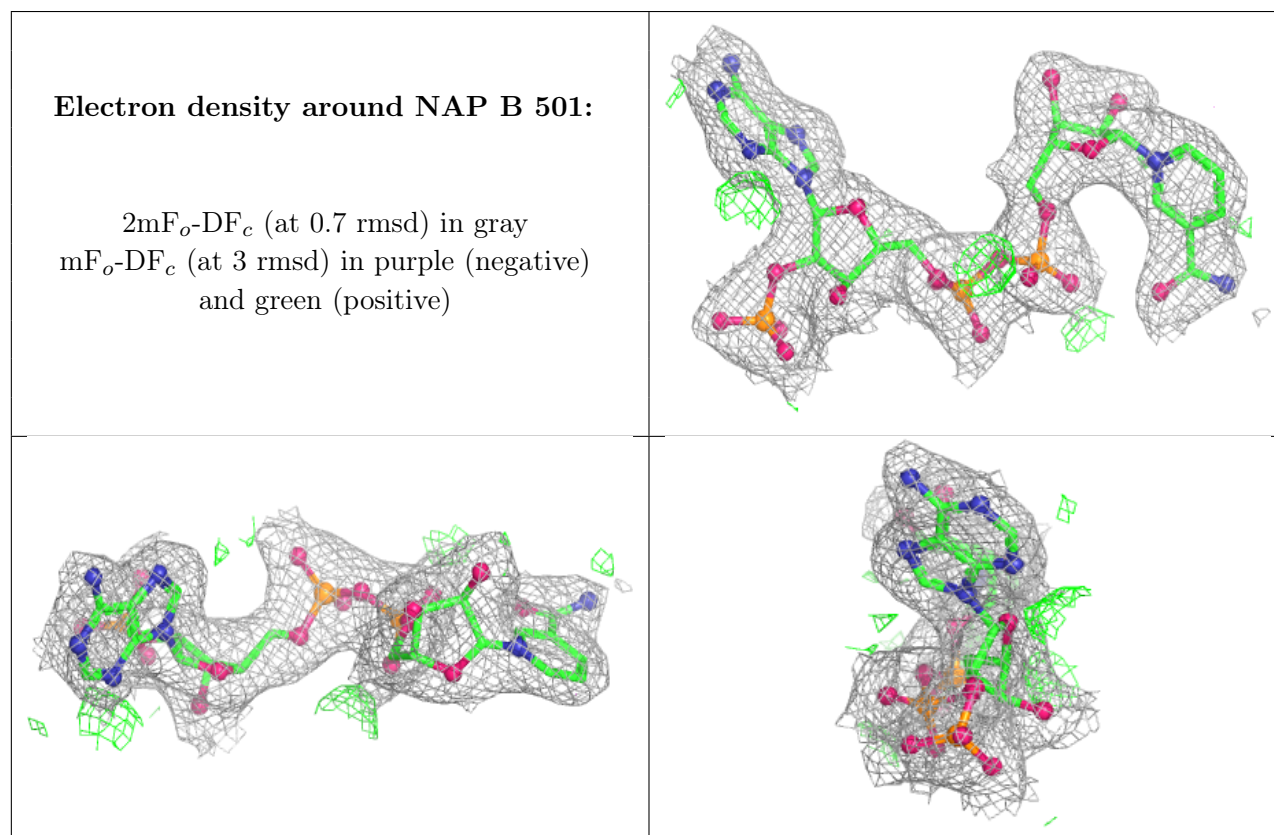
There are no oligosaccharides in this entry.

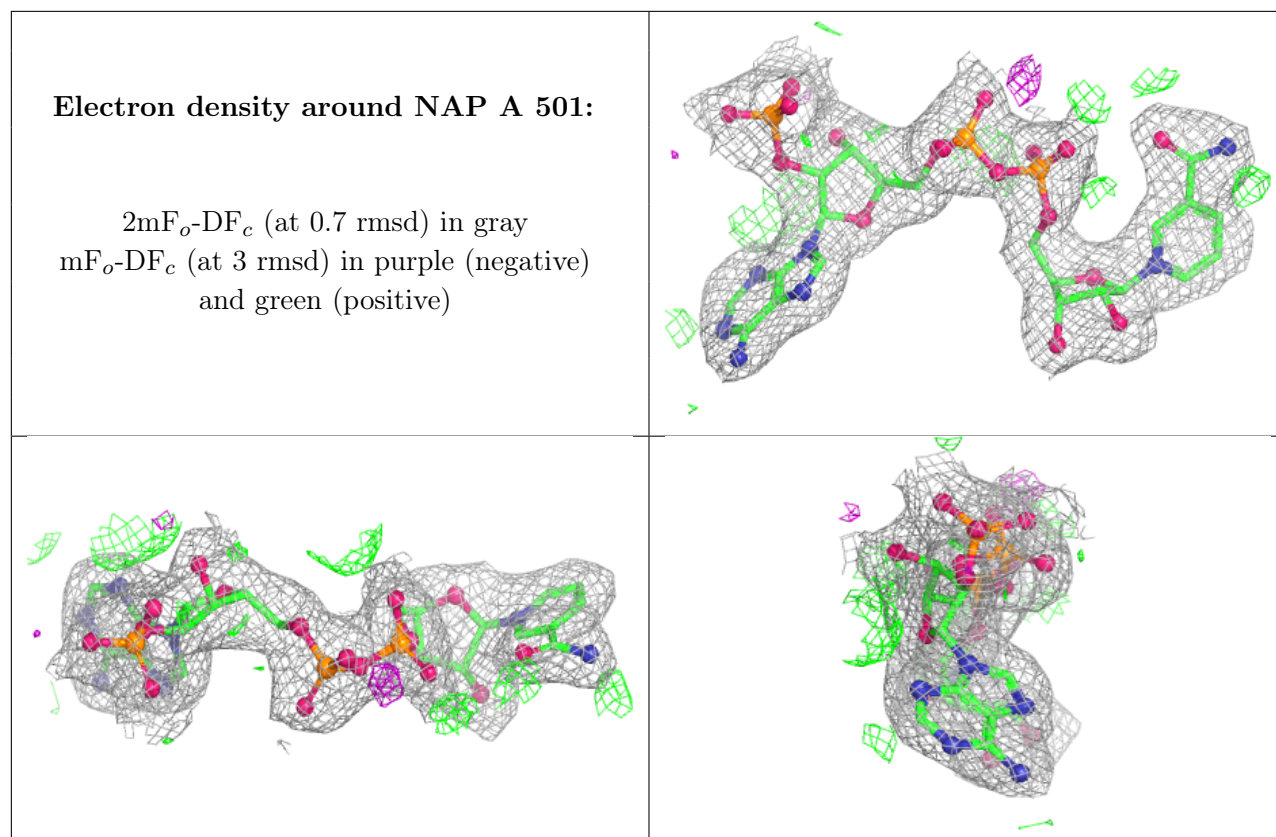
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	GOL	B	502	6/6	0.88	0.15	32,41,46,46	0
3	GOL	B	503	6/6	0.90	0.15	52,64,67,69	0
3	GOL	A	502	6/6	0.94	0.08	38,40,43,46	0
2	NAP	B	501	48/48	0.98	0.05	17,26,33,42	0
2	NAP	A	501	48/48	0.98	0.05	14,19,24,27	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.