WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 02:14 AM EST

PDB ID	:	8EP7
Title	:	Crystal Structure of the Ketol-acid Reductoisomerase from Bacillus anthracis in complex with NADP
Authors	:	Kim, Y.; Maltseva, N.; Osipiuk, J.; Gu, M.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID); Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on	:	2022-10-05
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

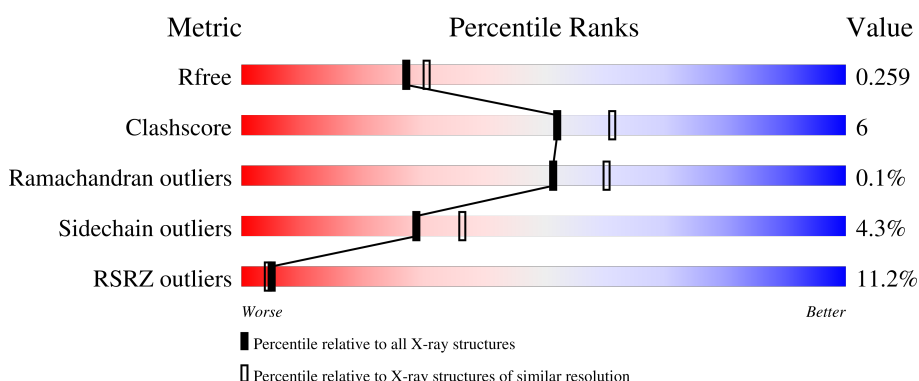|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.259
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		4.3%
RSRZ outliers		11.2%

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	335	12% / 80% 14% • 5%
1	B	335	18% / 75% 20% • •
1	C	335	% / 90% 8% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7881 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 Ketol-acid reductoisomerase (NADP(+)) 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	Se	0	0	0
			2461	1547	424	477	3	10			
1	B	323	Total	C	N	O	S	Se	0	0	0
			2500	1573	430	483	3	11			
1	C	328	Total	C	N	O	S	Se	0	3	0
			2563	1610	443	496	3	11			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).
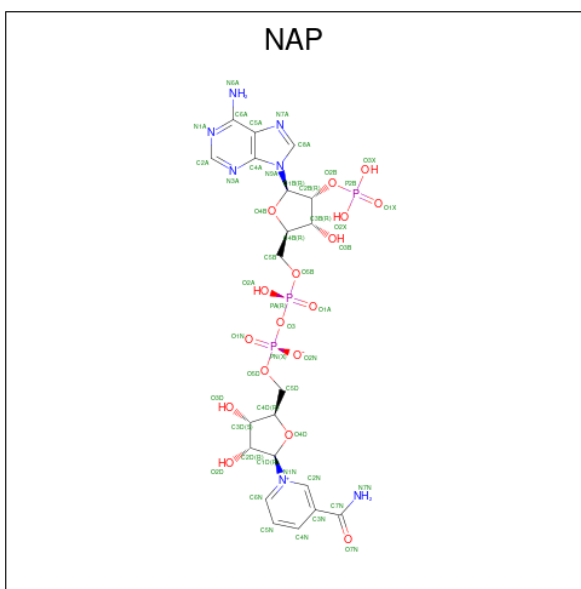
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).
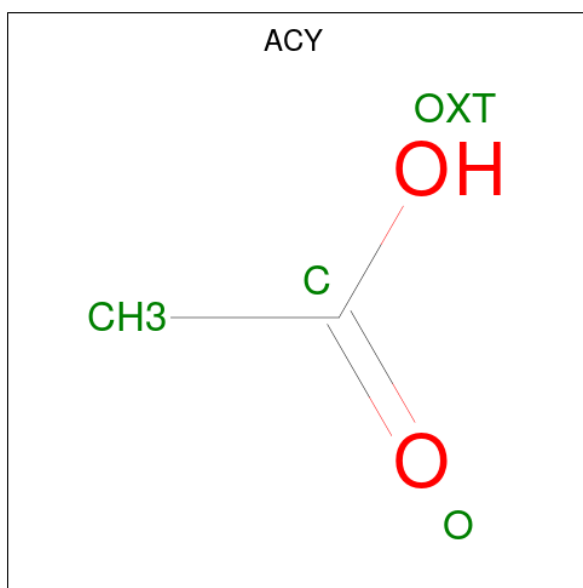
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total C O 4 2 2			0	0

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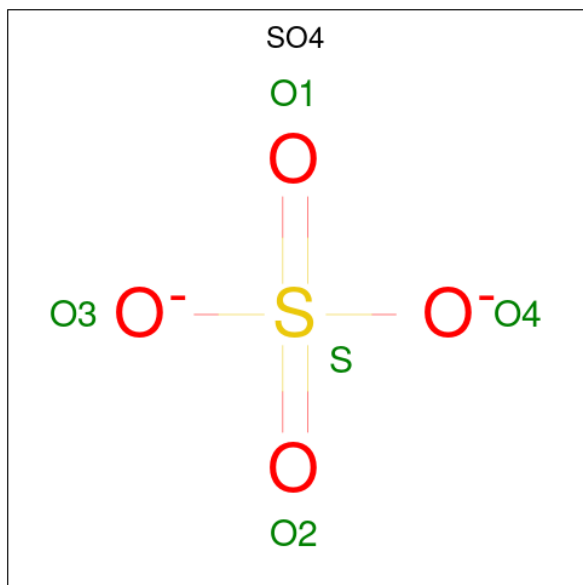
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total O S 5 4 1			0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total 45	O 45	0	0
5	B	36	Total 36	O 36	0	0
5	C	123	Total 123	O 123	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: Ketol-acid reductoisomerase (NADP(+)) 2
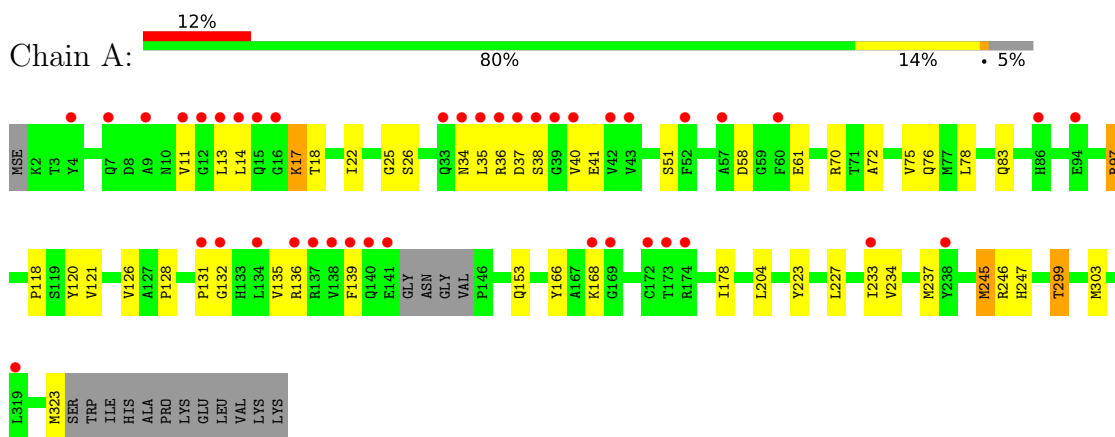
• Molecule 1: Ketol-acid reductoisomerase (NADP(+)) 2
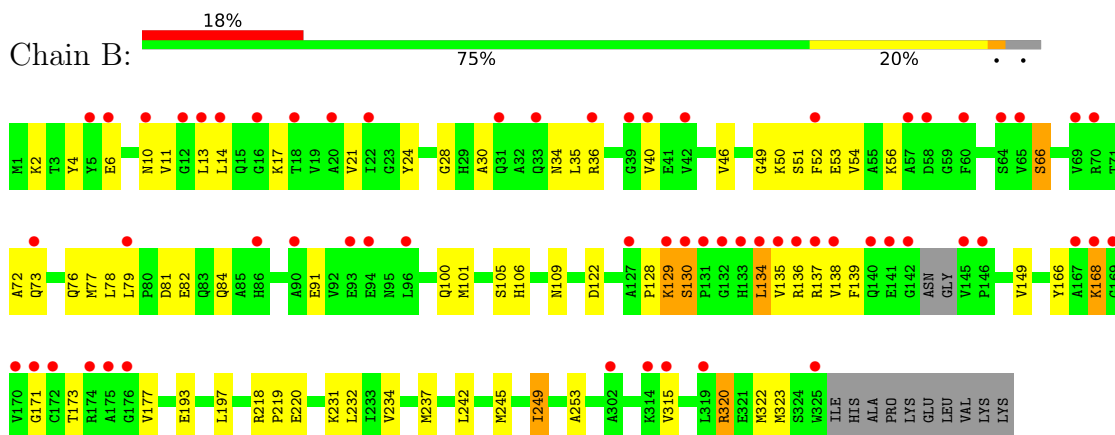
• Molecule 1: Ketol-acid reductoisomerase (NADP(+)) 2
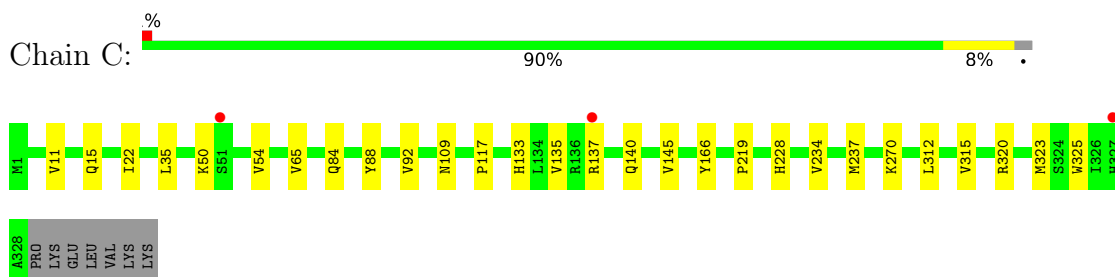
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.58Å　131.86Å　132.61Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	41.73　–　2.20 41.73　–　2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.73-2.20) 99.3 (41.73-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.93 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.217　,　0.262 0.216　,　0.259	Depositor DCC
R_{free} test set	2797 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.8	EDS
L-test for twinning[2]	$<|L|>$ = 0.47, $<L^2>$ = 0.29	Xtriage
Estimated twinning fraction	0.039 for -h,-l,-k 0.026 for l,-k,h 0.028 for -k,-h,-l 0.043 for k,-l,-h 0.043 for -l,h,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7881	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAP, ACY

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	0.29	0/2493	0.49	0/3349
1	B	0.29	0/2534	0.50	0/3406
1	C	0.32	0/2600	0.52	0/3497
All	All	0.30	0/7627	0.50	0/10252

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2461	0	2421	29	0
1	B	2500	0	2459	40	0
1	C	2563	0	2508	14	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	0	0
3	B	4	0	3	0	0
4	C	5	0	0	0	0
5	A	45	0	0	0	0
5	B	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	123	0	0	2	0
All	All	7881	0	7466	84	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 (84) 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:37:ASP:HB2	1:A:139:PHE:HE1	1.47	0.79
1:A:233:ILE:HD12	1:A:245:MSE:HE3	1.72	0.70
1:C:234:VAL:HA	1:C:237:MSE:HE2	1.80	0.64
1:B:21:VAL:HG13	1:B:78:LEU:HD12	1.79	0.63
1:B:30:ALA:HA	1:B:136:ARG:HB2	1.84	0.60
1:A:34:ASN:ND2	1:A:135:VAL:HG12	2.18	0.58
1:B:66:SER:HB2	1:B:91:GLU:HG2	1.83	0.58
1:B:52:PHE:CE1	1:B:56:LYS:HE2	2.39	0.58
1:B:234:VAL:HA	1:B:237:MSE:HE3	1.85	0.58
1:C:219:PRO:HB2	1:C:315:VAL:HG21	1.85	0.56
1:B:52:PHE:HE1	1:B:56:LYS:HE2	1.71	0.56
1:B:10:ASN:OD1	1:B:11:VAL:N	2.39	0.55
1:A:34:ASN:ND2	1:A:135:VAL:O	2.38	0.55
1:A:35:LEU:HD22	1:A:40:VAL:HG11	1.90	0.54
1:B:84:GLN:OE1	1:B:109:ASN:ND2	2.41	0.53
1:A:233:ILE:O	1:A:245:MSE:HG3	2.09	0.53
1:B:134:LEU:HA	1:B:137:ARG:HB2	1.90	0.53
1:B:76:GLN:HE21	1:B:77:MSE:H	1.54	0.53
1:A:121:VAL:O	1:A:153:GLN:NE2	2.41	0.52
1:A:11:VAL:HG23	1:A:168:LYS:HD3	1.91	0.52
1:A:299:THR:HG23	1:A:303:MSE:HE2	1.93	0.51
1:C:135:VAL:HG22	1:C:145:VAL:HG21	1.92	0.50
1:C:137:ARG:HA	1:C:140:GLN:HG2	1.92	0.50
1:A:35:LEU:HB3	1:A:40:VAL:HB	1.92	0.50
1:B:149:VAL:HG13	1:B:177:VAL:HG11	1.94	0.50
1:B:4:TYR:O	1:B:177:VAL:N	2.37	0.50
1:B:35:LEU:HD11	1:B:166:TYR:CE2	2.45	0.50
1:A:18:THR:OG1	1:A:72:ALA:HA	2.13	0.49
1:A:51:SER:OG	2:A:401:NAP:O2X	2.23	0.49
1:B:219:PRO:HB2	1:B:315:VAL:HG21	1.94	0.49
1:B:35:LEU:HD22	1:B:40:VAL:HG11	1.95	0.49
1:B:72:ALA:O	1:B:100:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG23	1:A:245:MSE:SE	2.64	0.48
1:B:218:ARG:NH2	1:B:220:GLU:OE1	2.40	0.48
1:C:133:HIS:HB2	5:C:610:HOH:O	2.13	0.48
1:B:320:ARG:HA	1:B:323:MSE:HE3	1.96	0.48
1:C:88:TYR:HA	1:C:92:VAL:HB	1.96	0.47
1:B:106:HIS:HB2	2:B:401:NAP:H1D	1.96	0.47
1:B:79:LEU:HB2	1:B:84:GLN:HG3	1.96	0.47
1:B:128:PRO:O	1:B:130:SER:N	2.47	0.47
1:C:228:HIS:HD2	5:C:524:HOH:O	1.98	0.47
1:B:168:LYS:HD2	1:B:173:THR:OG1	2.15	0.46
1:A:14:LEU:HA	1:A:17:LYS:HB2	1.97	0.46
1:A:34:ASN:OD1	1:A:136:ARG:HA	2.16	0.46
1:A:36:ARG:NH2	1:A:58:ASP:O	2.49	0.46
1:B:193:GLU:HA	1:B:197:LEU:HB2	1.97	0.46
1:B:81:ASP:HA	1:B:109:ASN:HD21	1.80	0.45
1:B:6:GLU:HG3	1:B:168:LYS:NZ	2.32	0.45
1:A:22:ILE:HD13	1:A:75:VAL:HG13	1.98	0.45
1:A:223:TYR:CE1	1:A:227:LEU:HD23	2.52	0.45
1:A:61:GLU:N	1:A:61:GLU:OE1	2.49	0.45
1:C:84:GLN:HB2	1:C:109:ASN:ND2	2.31	0.45
1:A:70:ARG:O	1:A:97:ARG:NH2	2.50	0.45
1:B:24:TYR:HA	1:B:28:GLY:HA3	1.99	0.45
1:C:50:LYS:O	1:C:54:VAL:HG23	2.17	0.45
1:C:88:TYR:OH	1:C:117:PRO:HA	2.17	0.44
1:A:131:PRO:O	1:A:135:VAL:HG23	2.18	0.44
1:A:35:LEU:HD11	1:A:166:TYR:CE2	2.52	0.44
1:C:234:VAL:HG22	1:C:237:MSE:HE2	1.99	0.43
1:B:76:GLN:HE21	1:B:77:MSE:N	2.16	0.43
1:B:249:ILE:HG13	1:B:253:ALA:HB3	1.99	0.43
1:C:35:LEU:HD11	1:C:166:TYR:CE2	2.54	0.43
1:A:126:VAL:O	1:A:128:PRO:HD3	2.18	0.43
1:C:22:ILE:HD12	1:C:65:VAL:HG13	2.01	0.42
1:C:320:ARG:HA	1:C:323:MSE:HE3	2.01	0.42
1:B:101:MSE:HA	1:B:122:ASP:HB2	2.00	0.42
1:B:49:GLY:O	1:B:53:GLU:HG2	2.19	0.42
1:B:46:VAL:HG13	1:B:52:PHE:CD2	2.54	0.42
1:A:26:SER:O	1:A:132:GLY:HA3	2.19	0.42
1:A:234:VAL:HG13	1:A:237:MSE:HE3	2.00	0.41
1:B:51:SER:HA	1:B:54:VAL:HB	2.01	0.41
1:A:25:GLY:HA3	2:A:401:NAP:O5B	2.20	0.41
1:B:106:HIS:CB	2:B:401:NAP:H1D	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:H	1:B:82:GLU:CD	2.24	0.41
1:B:139:PHE:CD2	1:B:171:GLY:HA3	2.55	0.41
1:A:76:GLN:HG3	1:A:78:LEU:HG	2.02	0.41
1:B:4:TYR:N	1:B:177:VAL:O	2.43	0.41
1:B:231:LYS:HD3	1:B:232:LEU:HD23	2.03	0.41
1:A:18:THR:HG22	1:A:41:GLU:HG2	2.03	0.40
2:B:401:NAP:H71N	2:B:401:NAP:H2N	1.68	0.40
1:B:134:LEU:HG	1:B:138:VAL:HG23	2.03	0.40
1:B:242:LEU:HA	1:B:242:LEU:HD23	1.81	0.40
1:B:34:ASN:ND2	1:B:135:VAL:O	2.38	0.40
1:A:118:PRO:HB2	1:A:120:TYR:CE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	314/335 (94%)	303 (96%)	11 (4%)	0	100	100
1	B	319/335 (95%)	300 (94%)	18 (6%)	1 (0%)	41	46
1	C	329/335 (98%)	320 (97%)	9 (3%)	0	100	100
All	All	962/1005 (96%)	923 (96%)	38 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	LYS

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	259/262 (99%)	247 (95%)	12 (5%)	27	34
1	B	263/262 (100%)	246 (94%)	17 (6%)	17	19
1	C	269/262 (103%)	264 (98%)	5 (2%)	57	71
All	All	791/786 (101%)	757 (96%)	34 (4%)	29	36

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	17	LYS
1	A	38	SER
1	A	83	GLN
1	A	97	ARG
1	A	178	ILE
1	A	204	LEU
1	A	245	MSE
1	A	246	ARG
1	A	247	HIS
1	A	299	THR
1	A	323	MSE
1	B	2	LYS
1	B	13	LEU
1	B	14	LEU
1	B	17	LYS
1	B	36	ARG
1	B	50	LYS
1	B	66	SER
1	B	73	GLN
1	B	105	SER
1	B	129	LYS
1	B	130	SER
1	B	134	LEU
1	B	168	LYS
1	B	245	MSE

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Mol	Chain	Res	Type
1	B	249	ILE
1	B	320	ARG
1	B	322	MSE
1	C	11	VAL
1	C	15	GLN
1	C	270	LYS
1	C	312	LEU
1	C	325	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	C	228	HIS

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 monosaccharides 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
2	NAP	C	401	-	45,52,52	2.75	12 (26%)	56,80,80	2.00	13 (23%)
2	NAP	B	401	-	45,52,52	2.65	10 (22%)	56,80,80	2.00	13 (23%)
4	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.08	0
2	NAP	A	401	-	45,52,52	2.80	12 (26%)	56,80,80	2.10	15 (26%)
3	ACY	B	402	-	3,3,3	1.05	0	3,3,3	0.51	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
2	NAP	C	401	-	-	8/31/67/67	0/5/5/5
2	NAP	B	401	-	-	14/31/67/67	0/5/5/5
2	NAP	A	401	-	-	21/31/67/67	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	P2B-O2B	13.66	1.85	1.59
2	C	401	NAP	P2B-O2B	13.28	1.84	1.59
2	B	401	NAP	P2B-O2B	12.48	1.82	1.59
2	B	401	NAP	C4N-C3N	5.99	1.49	1.39
2	A	401	NAP	C4N-C3N	5.97	1.49	1.39
2	C	401	NAP	C4N-C3N	5.76	1.49	1.39
2	C	401	NAP	C5N-C4N	5.00	1.49	1.38
2	A	401	NAP	C5N-C4N	4.93	1.49	1.38
2	B	401	NAP	C5N-C4N	4.57	1.48	1.38
2	B	401	NAP	PN-O5D	4.25	1.76	1.59
2	A	401	NAP	PN-O5D	3.92	1.75	1.59
2	C	401	NAP	C2N-N1N	3.54	1.39	1.35
2	A	401	NAP	C3N-C7N	-3.23	1.45	1.50
2	B	401	NAP	C7N-N7N	3.20	1.39	1.33
2	C	401	NAP	PN-O5D	3.18	1.72	1.59
2	B	401	NAP	C3N-C7N	-3.14	1.45	1.50
2	B	401	NAP	O2B-C2B	-3.02	1.33	1.44
2	A	401	NAP	C7N-N7N	3.01	1.38	1.33
2	A	401	NAP	C2N-N1N	2.97	1.38	1.35
2	C	401	NAP	O2B-C2B	-2.88	1.33	1.44
2	A	401	NAP	C2A-N1A	2.75	1.39	1.33
2	C	401	NAP	C3N-C7N	-2.72	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	C2A-N1A	2.71	1.39	1.33
2	A	401	NAP	O2B-C2B	-2.68	1.34	1.44
2	C	401	NAP	C7N-N7N	2.62	1.38	1.33
2	A	401	NAP	C4A-N3A	2.56	1.39	1.35
2	B	401	NAP	C6N-N1N	2.47	1.41	1.35
2	A	401	NAP	C6N-N1N	2.46	1.41	1.35
2	B	401	NAP	C2A-N1A	2.45	1.38	1.33
2	C	401	NAP	C4A-N3A	2.41	1.39	1.35
2	C	401	NAP	O5D-C5D	-2.08	1.36	1.44
2	B	401	NAP	C6N-C5N	-2.07	1.34	1.38
2	C	401	NAP	C6N-N1N	2.04	1.40	1.35
2	A	401	NAP	C2A-N3A	2.01	1.35	1.32

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAP	C5N-C4N-C3N	-7.31	111.69	120.34
2	B	401	NAP	C5N-C4N-C3N	-7.06	111.99	120.34
2	C	401	NAP	C5N-C4N-C3N	-6.61	112.52	120.34
2	A	401	NAP	PN-O3-PA	-6.55	110.34	132.83
2	C	401	NAP	PN-O3-PA	-6.43	110.76	132.83
2	B	401	NAP	PN-O3-PA	-6.19	111.58	132.83
2	A	401	NAP	O7N-C7N-C3N	4.55	125.08	119.63
2	B	401	NAP	O7N-C7N-C3N	3.99	124.41	119.63
2	C	401	NAP	O7N-C7N-C3N	3.78	124.16	119.63
2	B	401	NAP	C2N-C3N-C4N	3.76	122.52	118.26
2	A	401	NAP	C2N-C3N-C4N	3.56	122.29	118.26
2	C	401	NAP	O7N-C7N-N7N	-3.42	117.71	122.58
2	C	401	NAP	C2N-C3N-C4N	3.40	122.11	118.26
2	B	401	NAP	O2B-P2B-O1X	-3.21	96.99	109.39
2	A	401	NAP	O2B-P2B-O1X	-3.20	97.04	109.39
2	C	401	NAP	O2B-P2B-O1X	-3.04	97.67	109.39
2	B	401	NAP	PA-O5B-C5B	-3.02	103.98	121.68
2	A	401	NAP	C6N-N1N-C2N	-3.01	119.23	121.97
2	A	401	NAP	PA-O5B-C5B	-2.78	105.35	121.68
2	C	401	NAP	PA-O5B-C5B	-2.76	105.50	121.68
2	A	401	NAP	O5D-PN-O1N	-2.75	98.31	109.07
2	A	401	NAP	O2N-PN-O1N	2.73	125.73	112.24
2	B	401	NAP	O7N-C7N-N7N	-2.64	118.83	122.58
2	C	401	NAP	O3X-P2B-O2X	2.63	117.70	107.64
2	A	401	NAP	O3X-P2B-O2X	2.57	117.46	107.64
2	B	401	NAP	PN-O5D-C5D	-2.55	106.73	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAP	O3X-P2B-O2X	2.54	117.35	107.64
2	A	401	NAP	C3B-C2B-C1B	-2.50	98.20	102.89
2	A	401	NAP	O7N-C7N-N7N	-2.46	119.08	122.58
2	C	401	NAP	C6N-N1N-C2N	-2.45	119.74	121.97
2	B	401	NAP	O5D-PN-O1N	-2.38	99.75	109.07
2	A	401	NAP	O4B-C4B-C3B	2.31	109.68	105.11
2	C	401	NAP	O4B-C4B-C3B	2.30	109.67	105.11
2	B	401	NAP	O2N-PN-O1N	2.29	123.58	112.24
2	B	401	NAP	C6N-N1N-C2N	-2.21	119.96	121.97
2	B	401	NAP	C2A-N1A-C6A	-2.20	115.00	118.75
2	C	401	NAP	C6N-C5N-C4N	2.14	122.55	119.44
2	A	401	NAP	PN-O5D-C5D	-2.10	109.36	121.68
2	A	401	NAP	C2A-N1A-C6A	-2.05	115.25	118.75
2	C	401	NAP	O2N-PN-O5D	-2.01	98.42	107.75
2	C	401	NAP	O5D-PN-O1N	-2.01	101.23	109.07

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C2B-O2B-P2B-O1X
2	A	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	C5D-O5D-PN-O1N
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2D-C1D-N1N-C2N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	B	401	NAP	C5B-O5B-PA-O3
2	B	401	NAP	C3B-C4B-C5B-O5B
2	B	401	NAP	C5D-O5D-PN-O1N
2	B	401	NAP	C5D-O5D-PN-O2N
2	B	401	NAP	O4D-C4D-C5D-O5D
2	B	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	C2D-C1D-N1N-C6N
2	C	401	NAP	C2B-O2B-P2B-O1X
2	C	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	O4D-C4D-C5D-O5D
2	A	401	NAP	C3B-C4B-C5B-O5B
2	A	401	NAP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	B	401	NAP	C3D-C4D-C5D-O5D
2	B	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	PN-O3-PA-O1A
2	C	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	C5D-O5D-PN-O2N
2	B	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C2N-C3N-C7N-N7N
2	A	401	NAP	C2N-C3N-C7N-O7N
2	A	401	NAP	PN-O3-PA-O2A
2	A	401	NAP	PN-O3-PA-O1A
2	C	401	NAP	PN-O3-PA-O2A
2	A	401	NAP	C4N-C3N-C7N-N7N
2	C	401	NAP	C3B-C4B-C5B-O5B
2	B	401	NAP	C2B-O2B-P2B-O1X
2	A	401	NAP	C5B-O5B-PA-O3
2	B	401	NAP	C2D-C1D-N1N-C2N
2	C	401	NAP	C2B-O2B-P2B-O3X
2	C	401	NAP	C2D-C1D-N1N-C6N
2	A	401	NAP	C4N-C3N-C7N-O7N
2	A	401	NAP	C5B-O5B-PA-O2A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand NAP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 401

Bond lengths

Bond angles

Torsions

Rings
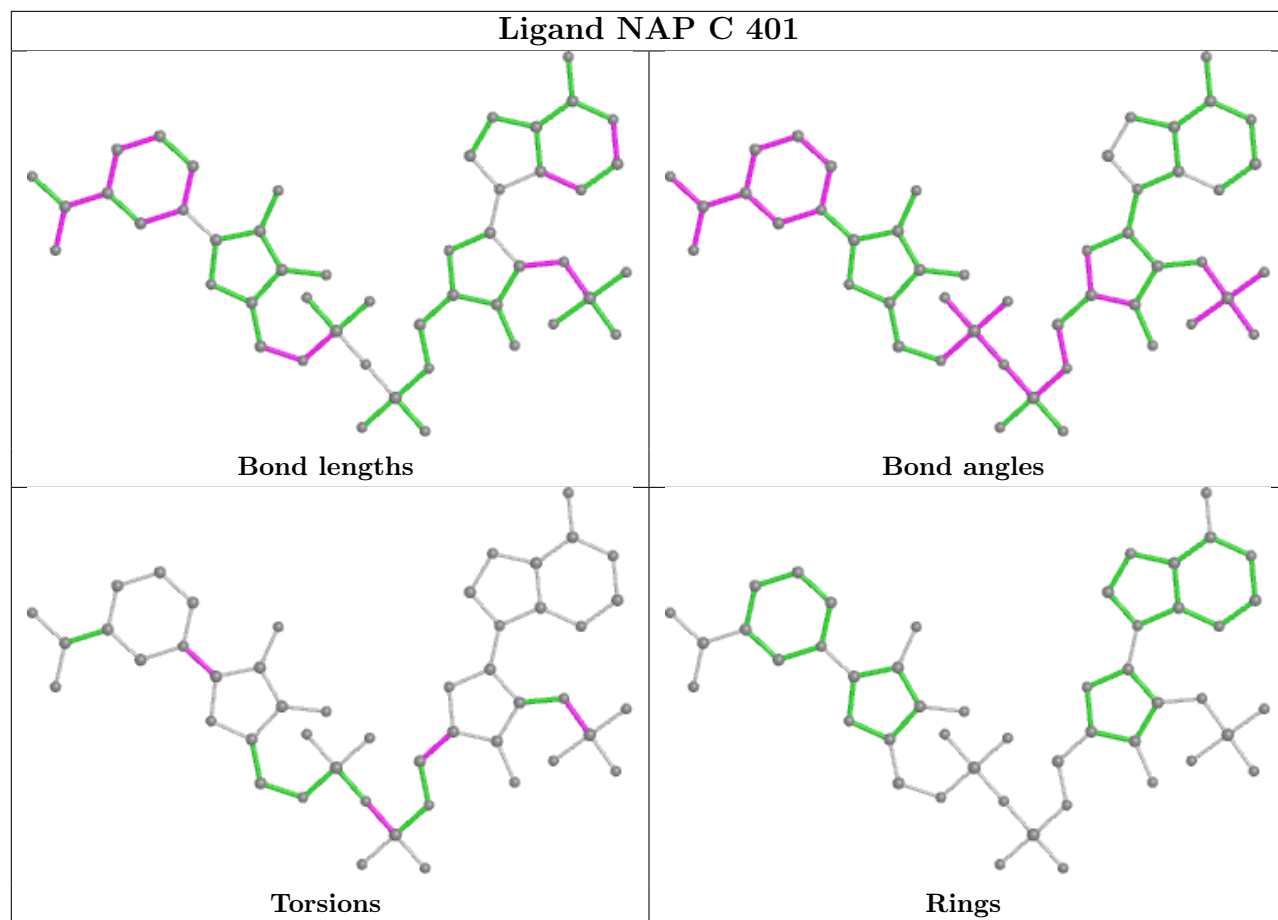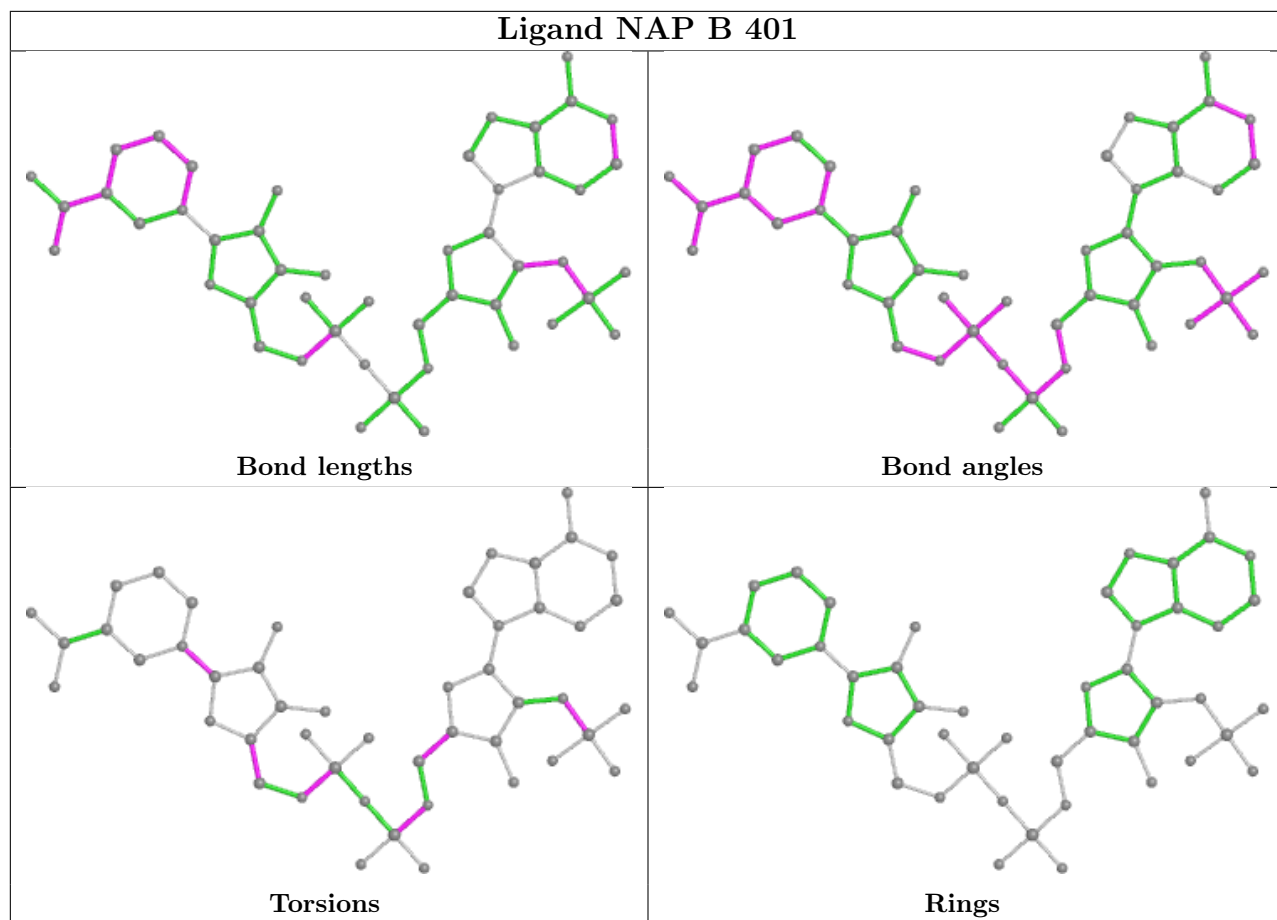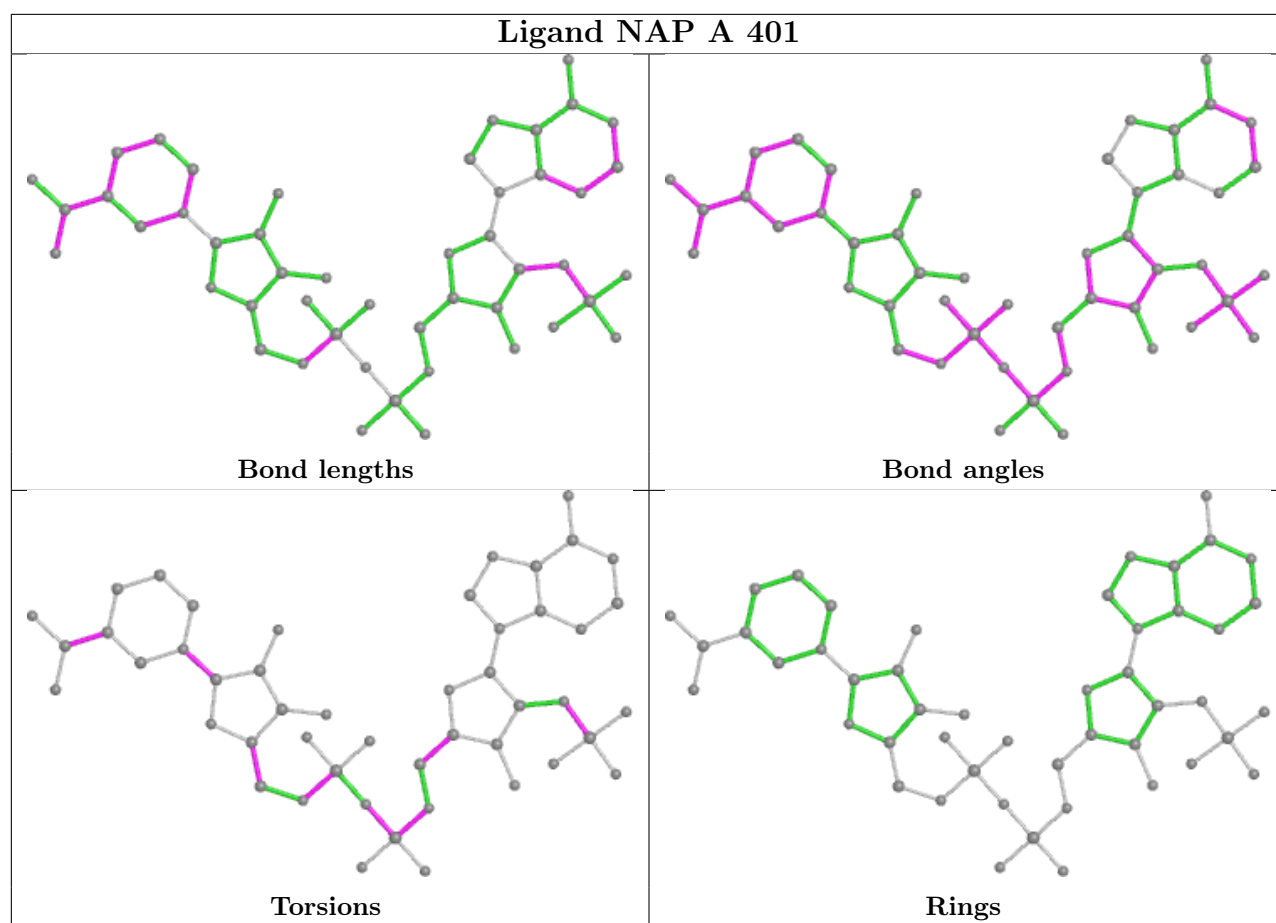
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	308/335 (91%)	0.70	41 (13%)	3	3	41, 76, 120, 164	1 (0%)
1	B	312/335 (93%)	1.05	61 (19%)	1	1	44, 79, 128, 172	11 (3%)
1	C	317/335 (94%)	-0.08	3 (0%)	84	83	28, 44, 72, 126	0
All	All	937/1005 (93%)	0.55	105 (11%)	5	4	28, 64, 119, 172	12 (1%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	GLY	8.5
1	B	5	TYR	8.3
1	B	40	VAL	8.1
1	B	60	PHE	7.6
1	B	175	ALA	7.0
1	A	16	GLY	5.9
1	B	174	ARG	5.7
1	B	325	TRP	5.6
1	A	139	PHE	5.6
1	A	11	VAL	5.5
1	A	43	VAL	5.2
1	A	137	ARG	4.8
1	B	10	ASN	4.7
1	A	36	ARG	4.6
1	B	176	GLY	4.6
1	A	37	ASP	4.5
1	B	170	VAL	4.4
1	A	140	GLN	4.4
1	B	141	GLU	4.3
1	B	13	LEU	4.3
1	A	174	ARG	4.2
1	B	130	SER	4.2
1	B	167	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	14	LEU	4.1
1	B	12	GLY	4.1
1	A	60	PHE	4.1
1	B	22	ILE	4.0
1	A	169	GLY	4.0
1	B	65	VAL	3.9
1	A	136	ARG	3.8
1	B	134	LEU	3.8
1	A	168	LYS	3.8
1	B	315	VAL	3.7
1	A	35	LEU	3.6
1	A	33	GLN	3.6
1	B	94	GLU	3.6
1	A	7	GLN	3.5
1	A	319	LEU	3.5
1	B	138	VAL	3.5
1	A	57	ALA	3.4
1	A	9	ALA	3.3
1	A	14	LEU	3.3
1	B	140	GLN	3.3
1	B	314	LYS	3.2
1	B	136	ARG	3.2
1	C	327	HIS	3.2
1	B	146	PRO	3.2
1	A	134	LEU	3.1
1	B	79	LEU	3.0
1	B	96	LEU	3.0
1	A	172	CYS	2.9
1	A	238	TYR	2.9
1	A	42	VAL	2.9
1	A	141	GLU	2.9
1	B	132	GLY	2.9
1	B	6	GLU	2.8
1	B	90	ALA	2.8
1	B	172	CYS	2.8
1	A	173	THR	2.8
1	B	137	ARG	2.8
1	A	40	VAL	2.7
1	B	145	VAL	2.7
1	A	15	GLN	2.7
1	B	20	ALA	2.7
1	B	129	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	38	SER	2.7
1	A	131	PRO	2.6
1	B	86	HIS	2.5
1	B	64	SER	2.5
1	B	135	VAL	2.5
1	B	57	ALA	2.5
1	A	4	TYR	2.5
1	B	70	ARG	2.4
1	A	39	GLY	2.4
1	B	169	GLY	2.4
1	B	319	LEU	2.4
1	A	138	VAL	2.4
1	B	31	GLN	2.4
1	A	233	ILE	2.4
1	B	39	GLY	2.4
1	A	52	PHE	2.4
1	B	73	GLN	2.4
1	A	12	GLY	2.3
1	B	33	GLN	2.3
1	A	86	HIS	2.3
1	B	127	ALA	2.3
1	B	58	ASP	2.3
1	B	42	VAL	2.3
1	A	94	GLU	2.3
1	A	13	LEU	2.2
1	B	168	LYS	2.2
1	B	36	ARG	2.2
1	B	16	GLY	2.2
1	C	51	SER	2.2
1	B	18	THR	2.2
1	B	133	HIS	2.1
1	C	137	ARG	2.1
1	A	34	ASN	2.1
1	B	93	GLU	2.1
1	B	131	PRO	2.1
1	B	69	VAL	2.1
1	A	132	GLY	2.1
1	B	142	GLY	2.0
1	B	302	ALA	2.0
1	B	52	PHE	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

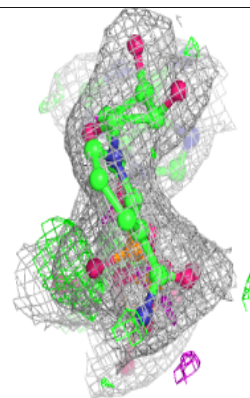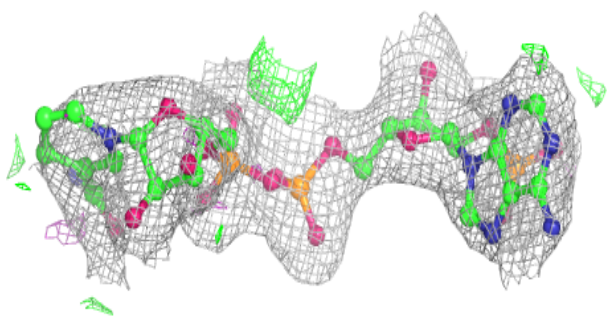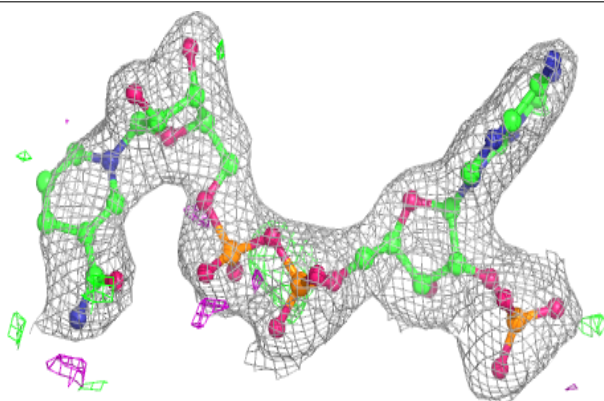| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	B	401	48/48	0.84	0.20	69,89,97,101	48
3	ACY	B	402	4/4	0.89	0.24	44,52,54,55	0
2	NAP	A	401	48/48	0.93	0.13	41,64,71,73	0
4	SO4	C	402	5/5	0.94	0.25	89,92,100,101	0
2	NAP	C	401	48/48	0.95	0.13	31,44,62,66	0

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.
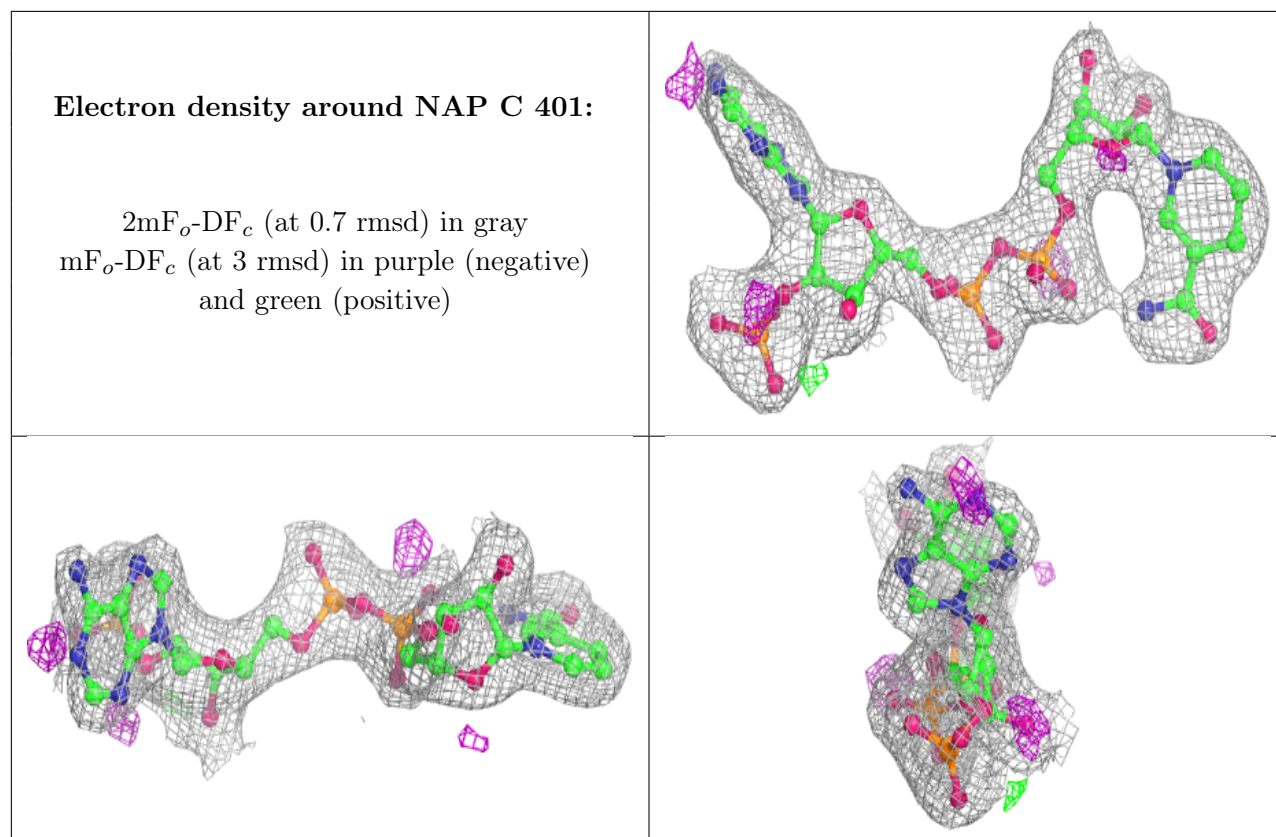
Electron density around NAP B 401:

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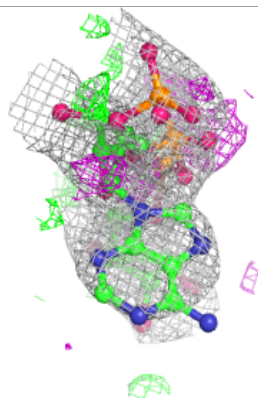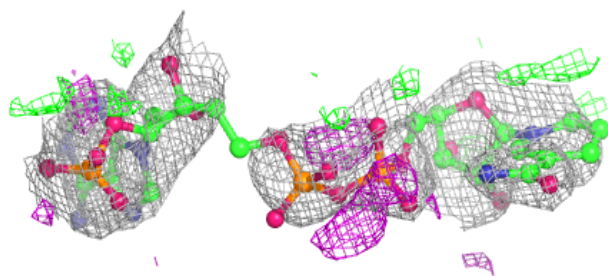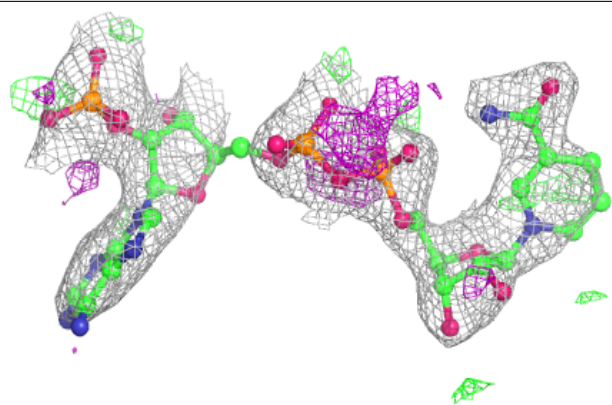
Electron density around NAP A 401:

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

Electron density around NAP C 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.