



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:30 PM UTC

PDB ID : 6ZN7 / pdb_00006zn7
Title : MaeB malic enzyme domain apoprotein
Authors : Lovering, A.L.; Harding, C.J.
Deposited on : 2020-07-06
Resolution : 1.67 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

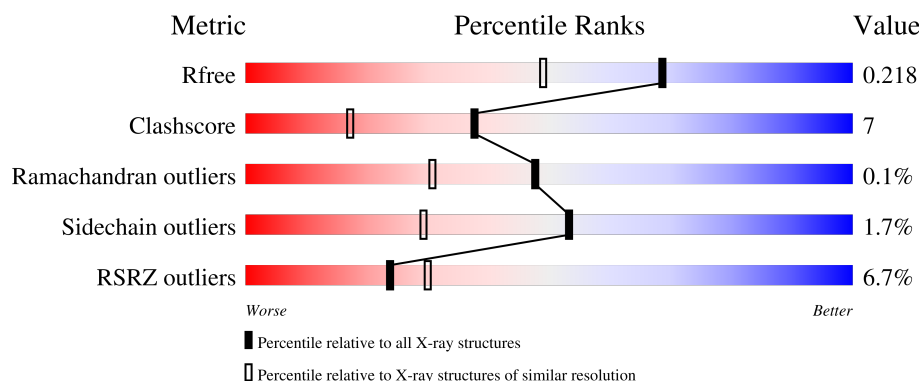
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	445	7% 78% 13% • 9%
1	B	445	6% 78% 12% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6864 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 NADP-dependent malate dehydrogenase, Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	2	0
			3053	1933	524	579	17			
1	B	411	Total	C	N	O	S	0	0	0
			3096	1961	531	587	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q6MM14
A	-9	GLY	-	expression tag	UNP Q6MM14
A	-8	SER	-	expression tag	UNP Q6MM14
A	-7	SER	-	expression tag	UNP Q6MM14
A	-6	HIS	-	expression tag	UNP Q6MM14
A	-5	HIS	-	expression tag	UNP Q6MM14
A	-4	HIS	-	expression tag	UNP Q6MM14
A	-3	HIS	-	expression tag	UNP Q6MM14
A	-2	HIS	-	expression tag	UNP Q6MM14
A	-1	HIS	-	expression tag	UNP Q6MM14
A	0	SER	-	expression tag	UNP Q6MM14
A	121	ASP	-	linker	UNP Q6MM14
A	122	ILE	-	linker	UNP Q6MM14
A	123	GLU	-	linker	UNP Q6MM14
A	124	VAL	-	linker	UNP Q6MM14
B	-10	MET	-	initiating methionine	UNP Q6MM14
B	-9	GLY	-	expression tag	UNP Q6MM14
B	-8	SER	-	expression tag	UNP Q6MM14
B	-7	SER	-	expression tag	UNP Q6MM14
B	-6	HIS	-	expression tag	UNP Q6MM14
B	-5	HIS	-	expression tag	UNP Q6MM14
B	-4	HIS	-	expression tag	UNP Q6MM14
B	-3	HIS	-	expression tag	UNP Q6MM14
B	-2	HIS	-	expression tag	UNP Q6MM14

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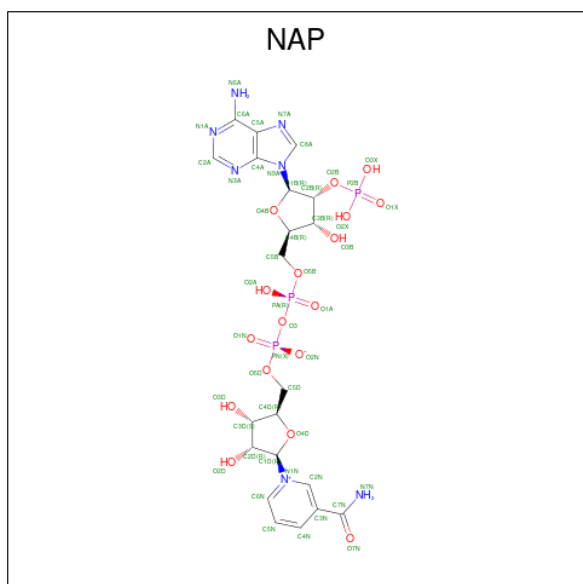
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP Q6MM14
B	0	SER	-	expression tag	UNP Q6MM14
B	121	ASP	-	linker	UNP Q6MM14
B	122	ILE	-	linker	UNP Q6MM14
B	123	GLU	-	linker	UNP Q6MM14
B	124	VAL	-	linker	UNP Q6MM14

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



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

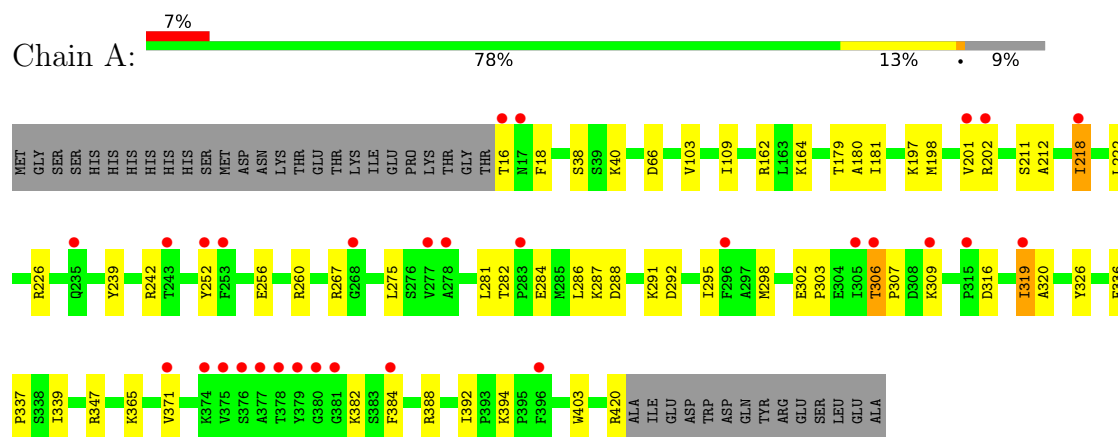
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total 248	O 248	0	0
4	B	369	Total 369	O 369	0	0

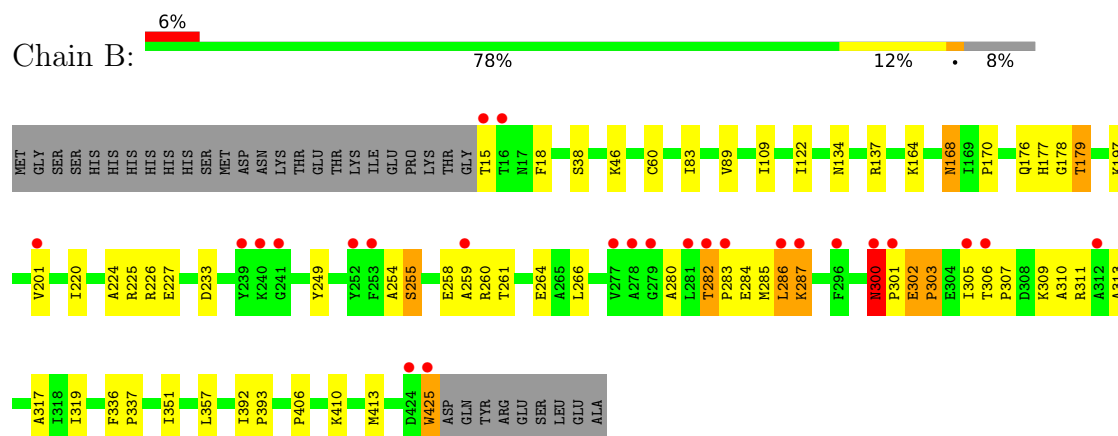
3 Residue-property plots

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: NADP-dependent malate dehydrogenase, Malate dehydrogenase



- Molecule 1: NADP-dependent malate dehydrogenase, Malate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.82Å 92.19Å 95.80Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	95.78 – 1.67 95.78 – 1.67	Depositor EDS
% Data completeness (in resolution range)	97.7 (95.78-1.67) 97.8 (95.78-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.179 , 0.218 0.183 , 0.218	Depositor DCC
R_{free} test set	4885 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k 0.022 for -h,-l,-k 0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6864	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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, MG

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	0.57	3/3113 (0.1%)	0.77	0/4216
1	B	0.78	6/3152 (0.2%)	0.94	10/4269 (0.2%)
All	All	0.68	9/6265 (0.1%)	0.86	10/8485 (0.1%)

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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	GLY	C-O	-6.88	1.15	1.23
1	A	40	LYS	C-O	-6.78	1.17	1.24
1	B	179	THR	N-CA	-6.06	1.39	1.46
1	B	89	VAL	C-O	-5.93	1.17	1.24
1	B	176	GLN	C-O	-5.85	1.18	1.23
1	B	302	GLU	C-N	5.27	1.40	1.33
1	A	164	LYS	C-O	-5.18	1.18	1.24
1	B	233	ASP	C-O	-5.15	1.19	1.24
1	A	211	SER	C-O	-5.10	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ASN	CA-C-N	-12.36	104.39	119.84
1	B	300	ASN	C-N-CA	-12.36	104.39	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ASN	CB-CA-C	9.75	129.38	110.17
1	B	287	LYS	N-CA-C	8.99	123.26	111.75
1	B	282	THR	CA-C-N	7.49	128.16	119.47
1	B	282	THR	C-N-CA	7.49	128.16	119.47
1	B	177	HIS	N-CA-C	7.24	122.21	113.23
1	B	286	LEU	N-CA-C	7.21	119.14	111.28
1	B	303	PRO	N-CA-C	6.46	120.26	111.22
1	B	425	TRP	N-CA-C	6.41	128.93	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	ASN	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	3053	0	3098	42	0
1	B	3096	0	3132	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	48	0	23	1	0
3	B	48	0	23	0	0
4	A	248	0	0	9	1
4	B	369	0	0	10	1
All	All	6864	0	6276	88	2

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 7.

All (88) 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:B:261:THR:HG23	1:B:264:GLU:H	1.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66[B]:ASP:OD1	4:A:901:HOH:O	1.89	0.88
1:B:307:PRO:HA	1:B:319:ILE:HD13	1.56	0.86
1:B:249:TYR:OH	4:B:901:HOH:O	1.97	0.81
1:B:15:THR:HG23	1:B:18:PHE:HB3	1.68	0.76
1:A:388:ARG:HD3	4:A:906:HOH:O	1.87	0.74
1:A:284:GLU:N	4:A:903:HOH:O	2.22	0.71
1:A:282:THR:OG1	4:A:903:HOH:O	2.09	0.70
1:A:307:PRO:HA	1:A:319:ILE:HD12	1.73	0.70
1:A:181:ILE:HD13	1:A:339:ILE:HD11	1.74	0.68
1:B:425:TRP:C	4:B:1118:HOH:O	2.40	0.65
1:B:282:THR:H	1:B:285:MET:HE3	1.61	0.65
1:A:38:SER:HB2	1:B:109:ILE:HD12	1.78	0.64
1:A:347:ARG:HD2	1:A:420:ARG:HB2	1.78	0.64
1:B:254:ALA:O	4:B:902:HOH:O	2.15	0.64
1:B:197:LYS:O	1:B:201:VAL:HG23	1.98	0.63
1:B:309:LYS:HA	1:B:309:LYS:HE2	1.81	0.63
1:B:46:LYS:NZ	4:B:908:HOH:O	2.34	0.61
1:A:371:VAL:HG21	1:A:384:PHE:HB2	1.83	0.60
1:B:137:ARG:NH2	4:B:909:HOH:O	2.34	0.60
1:B:261:THR:HG23	1:B:264:GLU:N	2.09	0.60
1:A:197:LYS:O	1:A:201:VAL:HG23	2.01	0.60
1:A:306:THR:OG1	1:A:309:LYS:HG3	2.01	0.60
1:A:282:THR:C	4:A:903:HOH:O	2.46	0.59
1:B:311:ARG:NH1	1:B:317:ALA:O	2.35	0.59
1:B:261:THR:HG22	1:B:264:GLU:CD	2.30	0.57
1:A:162:ARG:HD3	4:A:1102:HOH:O	2.05	0.56
1:A:307:PRO:HA	1:A:319:ILE:CD1	2.36	0.55
1:B:220:ILE:HD13	1:B:226:ARG:HG2	1.89	0.54
1:A:382:LYS:NZ	4:A:911:HOH:O	2.39	0.54
1:A:16:THR:HG22	1:A:18:PHE:H	1.74	0.53
1:B:261:THR:HG22	1:B:264:GLU:CG	2.39	0.53
1:B:164:LYS:O	4:B:904:HOH:O	2.18	0.53
1:B:225:ARG:HB3	1:B:227:GLU:OE1	2.08	0.53
1:A:292:ASP:HA	1:A:316:ASP:O	2.08	0.52
1:B:259:ALA:O	1:B:260:ARG:HD2	2.10	0.52
1:A:239:TYR:CZ	1:A:242:ARG:HB2	2.45	0.52
1:A:287:LYS:HE2	1:A:288:ASP:OD1	2.10	0.51
1:A:298:MET:O	3:A:802:NAP:H2N	2.11	0.50
1:B:305:ILE:CG1	1:B:306:THR:N	2.74	0.50
1:A:103:VAL:HG23	1:B:60:CYS:SG	2.52	0.50
1:B:392:ILE:HG13	1:B:393:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASN:ND2	4:B:914:HOH:O	2.45	0.49
1:A:218:ILE:O	1:A:222:LEU:HG	2.13	0.49
1:B:410:LYS:HA	1:B:413:MET:HE3	1.95	0.49
1:A:336:PHE:CG	1:A:337:PRO:HD3	2.49	0.48
1:B:227:GLU:H	1:B:227:GLU:CD	2.20	0.48
1:B:305:ILE:HG12	1:B:306:THR:N	2.30	0.47
1:A:256:GLU:HG2	4:A:936:HOH:O	2.14	0.47
1:B:336:PHE:CG	1:B:337:PRO:HD3	2.49	0.47
1:A:281:LEU:HD21	1:A:286:LEU:HD21	1.95	0.47
1:B:170:PRO:HB3	1:B:351:ILE:HG13	1.96	0.47
1:A:307:PRO:HG2	1:A:326:TYR:CD1	2.51	0.46
1:A:181:ILE:HD13	1:A:339:ILE:CD1	2.43	0.45
1:A:365:LYS:HE3	1:A:403:TRP:HZ3	1.82	0.45
1:A:180:ALA:HB1	1:A:218:ILE:HG13	1.99	0.45
1:A:212:ALA:HA	1:A:275:LEU:CD1	2.47	0.45
1:B:300:ASN:C	1:B:302:GLU:N	2.74	0.45
1:B:286:LEU:N	1:B:286:LEU:CD1	2.79	0.44
1:A:109:ILE:HD12	1:B:38:SER:HB2	2.00	0.44
1:B:261:THR:CG2	1:B:264:GLU:H	2.14	0.44
1:A:394:LYS:NZ	4:A:914:HOH:O	2.45	0.43
1:B:303:PRO:HB2	1:B:305:ILE:O	2.18	0.43
1:B:258:GLU:CD	1:B:258:GLU:N	2.76	0.43
1:A:198:MET:HE2	1:A:222:LEU:HB2	2.00	0.43
1:B:282:THR:N	1:B:285:MET:HE3	2.31	0.43
1:A:239:TYR:CE1	1:A:242:ARG:HB2	2.54	0.43
1:A:202:ARG:NH2	1:A:267:ARG:O	2.52	0.43
1:A:302:GLU:HA	1:A:303:PRO:HD3	1.89	0.43
1:B:83:ILE:HG12	1:B:122:ILE:HB	2.02	0.42
1:A:226:ARG:NH2	1:A:252:TYR:O	2.40	0.42
1:A:291:LYS:NZ	1:A:292:ASP:OD2	2.52	0.42
1:B:310:ALA:HB3	1:B:319:ILE:CD1	2.50	0.42
1:B:286:LEU:HA	1:B:286:LEU:HD12	1.76	0.42
1:A:286:LEU:HD22	1:A:295:ILE:HD11	2.02	0.41
1:B:224:ALA:O	4:B:905:HOH:O	2.22	0.41
1:B:282:THR:HB	1:B:283:PRO:HD2	2.03	0.41
1:A:319:ILE:HG12	1:A:320:ALA:N	2.33	0.41
1:B:287:LYS:HE3	1:B:313:ALA:HB1	2.02	0.41
1:B:255:SER:HB2	4:B:1059:HOH:O	2.21	0.41
1:B:305:ILE:CG1	1:B:306:THR:H	2.34	0.41
1:B:309:LYS:HA	1:B:309:LYS:CE	2.50	0.41
1:B:197:LYS:N	1:B:197:LYS:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:HA	1:B:301:PRO:HA	1.85	0.40
1:B:134:ASN:ND2	4:B:919:HOH:O	2.49	0.40
1:B:406:PRO:O	1:B:410:LYS:HG3	2.21	0.40
1:A:260:ARG:HD3	1:A:260:ARG:HA	1.89	0.40
1:A:292:ASP:CG	1:A:388:ARG:HH22	2.29	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1076:HOH:O	4:B:1158:HOH:O[2_757]	2.12	0.08
4:A:1065:HOH:O	4:A:1087:HOH:O[1_655]	2.15	0.05

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	405/445 (91%)	394 (97%)	11 (3%)	0	100	100
1	B	409/445 (92%)	391 (96%)	17 (4%)	1 (0%)	43	27
All	All	814/890 (92%)	785 (96%)	28 (3%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ALA

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	320/354 (90%)	315 (98%)	5 (2%)	55	32
1	B	323/354 (91%)	317 (98%)	6 (2%)	50	25
All	All	643/708 (91%)	632 (98%)	11 (2%)	53	29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	A	218	ILE
1	A	306	THR
1	A	319	ILE
1	A	392	ILE
1	B	168	ASN
1	B	179	THR
1	B	255	SER
1	B	266	LEU
1	B	284	GLU
1	B	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	176	GLN
1	A	332	ASN
1	A	350	GLN
1	B	27	GLN
1	B	168	ASN
1	B	176	GLN
1	B	206	ASN
1	B	332	ASN

5.3.3 RNA ⓘ

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, 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	$\# Z > 2$
3	NAP	B	802	-	50,52,52	3.46	23 (46%)	71,80,80	1.83	16 (22%)
3	NAP	A	802	-	50,52,52	3.65	23 (46%)	71,80,80	1.92	17 (23%)

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	NAP	B	802	-	-	5/35/67/67	0/5/5/5
3	NAP	A	802	-	-	7/35/67/67	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	NAP	O4D-C1D	12.97	1.57	1.40
3	B	802	NAP	O4D-C1D	12.74	1.57	1.40
3	B	802	NAP	C2B-C1B	-9.35	1.30	1.53
3	A	802	NAP	C2B-C1B	-9.28	1.30	1.53
3	A	802	NAP	PN-O3	-8.44	1.50	1.59
3	A	802	NAP	O4B-C1B	7.53	1.59	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	NAP	O4D-C4D	-7.30	1.28	1.45
3	A	802	NAP	O4D-C4D	-7.24	1.28	1.45
3	B	802	NAP	O4B-C4B	-6.82	1.29	1.45
3	B	802	NAP	O4B-C1B	6.78	1.57	1.42
3	A	802	NAP	O4B-C4B	-6.52	1.30	1.45
3	B	802	NAP	O3B-C3B	-5.05	1.30	1.43
3	A	802	NAP	O3B-C3B	-4.46	1.31	1.43
3	A	802	NAP	P2B-O2B	-4.29	1.52	1.59
3	B	802	NAP	C7N-N7N	4.04	1.40	1.33
3	B	802	NAP	P2B-O2B	-3.96	1.52	1.59
3	B	802	NAP	O3D-C3D	-3.70	1.33	1.43
3	A	802	NAP	O7N-C7N	-3.69	1.17	1.24
3	A	802	NAP	C7N-N7N	3.57	1.39	1.33
3	A	802	NAP	O2D-C2D	3.37	1.51	1.43
3	A	802	NAP	P2B-O2X	-3.37	1.42	1.54
3	B	802	NAP	O2D-C2D	3.27	1.51	1.43
3	A	802	NAP	C6A-N6A	3.12	1.42	1.34
3	B	802	NAP	C6A-N6A	3.03	1.42	1.34
3	A	802	NAP	P2B-O3X	-2.98	1.43	1.54
3	A	802	NAP	PA-O3	-2.96	1.56	1.59
3	B	802	NAP	C5A-N7A	-2.96	1.33	1.39
3	B	802	NAP	O7N-C7N	-2.95	1.18	1.24
3	B	802	NAP	PN-O3	-2.80	1.56	1.59
3	B	802	NAP	P2B-O2X	-2.78	1.44	1.54
3	B	802	NAP	C2N-C3N	-2.77	1.34	1.39
3	B	802	NAP	C5D-C4D	2.73	1.59	1.51
3	B	802	NAP	C5A-C4A	-2.62	1.34	1.39
3	A	802	NAP	O3D-C3D	-2.59	1.36	1.43
3	B	802	NAP	C8A-N9A	-2.53	1.33	1.37
3	B	802	NAP	P2B-O3X	-2.51	1.45	1.54
3	A	802	NAP	C2N-N1N	2.47	1.37	1.35
3	A	802	NAP	C4N-C3N	-2.47	1.35	1.39
3	B	802	NAP	PA-O2A	-2.39	1.44	1.55
3	A	802	NAP	C5A-C4A	-2.35	1.34	1.39
3	A	802	NAP	C8A-N7A	2.34	1.36	1.31
3	A	802	NAP	PA-O2A	-2.31	1.44	1.55
3	A	802	NAP	PN-O1N	-2.27	1.42	1.50
3	A	802	NAP	C2A-N3A	2.14	1.37	1.33
3	B	802	NAP	C4N-C3N	-2.01	1.36	1.39
3	B	802	NAP	C5N-C4N	-2.00	1.35	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAP	N6A-C6A-N1A	-5.62	105.85	118.38
3	B	802	NAP	N6A-C6A-N1A	-5.52	106.08	118.38
3	A	802	NAP	N3A-C2A-N1A	-5.11	120.85	128.58
3	B	802	NAP	C5A-C4A-N3A	-4.88	120.00	126.72
3	A	802	NAP	C6N-N1N-C2N	-4.85	117.75	121.88
3	A	802	NAP	N9A-C8A-N7A	-4.74	107.21	113.94
3	B	802	NAP	C5A-C6A-N6A	4.68	134.86	123.29
3	B	802	NAP	N3A-C2A-N1A	-4.63	121.57	128.58
3	A	802	NAP	C5A-C4A-N3A	-4.52	120.50	126.72
3	A	802	NAP	C5A-C6A-N6A	4.45	134.31	123.29
3	B	802	NAP	N9A-C8A-N7A	-3.65	108.76	113.94
3	A	802	NAP	C5A-N7A-C8A	3.40	108.80	103.45
3	A	802	NAP	C4A-N9A-C1B	-3.13	119.31	126.63
3	A	802	NAP	C2A-N3A-C4A	3.11	119.42	111.83
3	B	802	NAP	C2A-N3A-C4A	2.99	119.14	111.83
3	B	802	NAP	C4D-O4D-C1D	-2.96	107.22	109.92
3	B	802	NAP	O3D-C3D-C2D	-2.89	102.56	111.82
3	B	802	NAP	C5A-C4A-N9A	2.79	108.85	105.81
3	B	802	NAP	C5A-N7A-C8A	2.71	107.71	103.45
3	B	802	NAP	O4B-C1B-C2B	-2.67	102.00	106.59
3	A	802	NAP	O7N-C7N-N7N	-2.65	118.79	122.62
3	B	802	NAP	C4A-C5A-N7A	-2.61	107.60	110.58
3	A	802	NAP	C1B-N9A-C8A	2.59	132.85	127.09
3	B	802	NAP	C6A-C5A-C4A	2.54	120.64	117.18
3	A	802	NAP	C4A-C5A-N7A	-2.49	107.73	110.58
3	A	802	NAP	C4D-O4D-C1D	-2.45	107.68	109.92
3	A	802	NAP	C5A-C4A-N9A	2.40	108.43	105.81
3	B	802	NAP	N3A-C4A-N9A	2.33	131.12	127.17
3	B	802	NAP	O2D-C2D-C3D	-2.31	104.40	111.82
3	A	802	NAP	O4B-C1B-C2B	-2.30	102.63	106.59
3	A	802	NAP	N3A-C4A-N9A	2.30	131.08	127.17
3	B	802	NAP	C6N-N1N-C2N	-2.29	119.93	121.88
3	A	802	NAP	C6A-C5A-C4A	2.04	119.97	117.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	NAP	O4D-C1D-N1N-C6N
3	A	802	NAP	C3B-C2B-O2B-P2B
3	B	802	NAP	C3B-C2B-O2B-P2B
3	B	802	NAP	O4B-C4B-C5B-O5B
3	B	802	NAP	C3B-C4B-C5B-O5B

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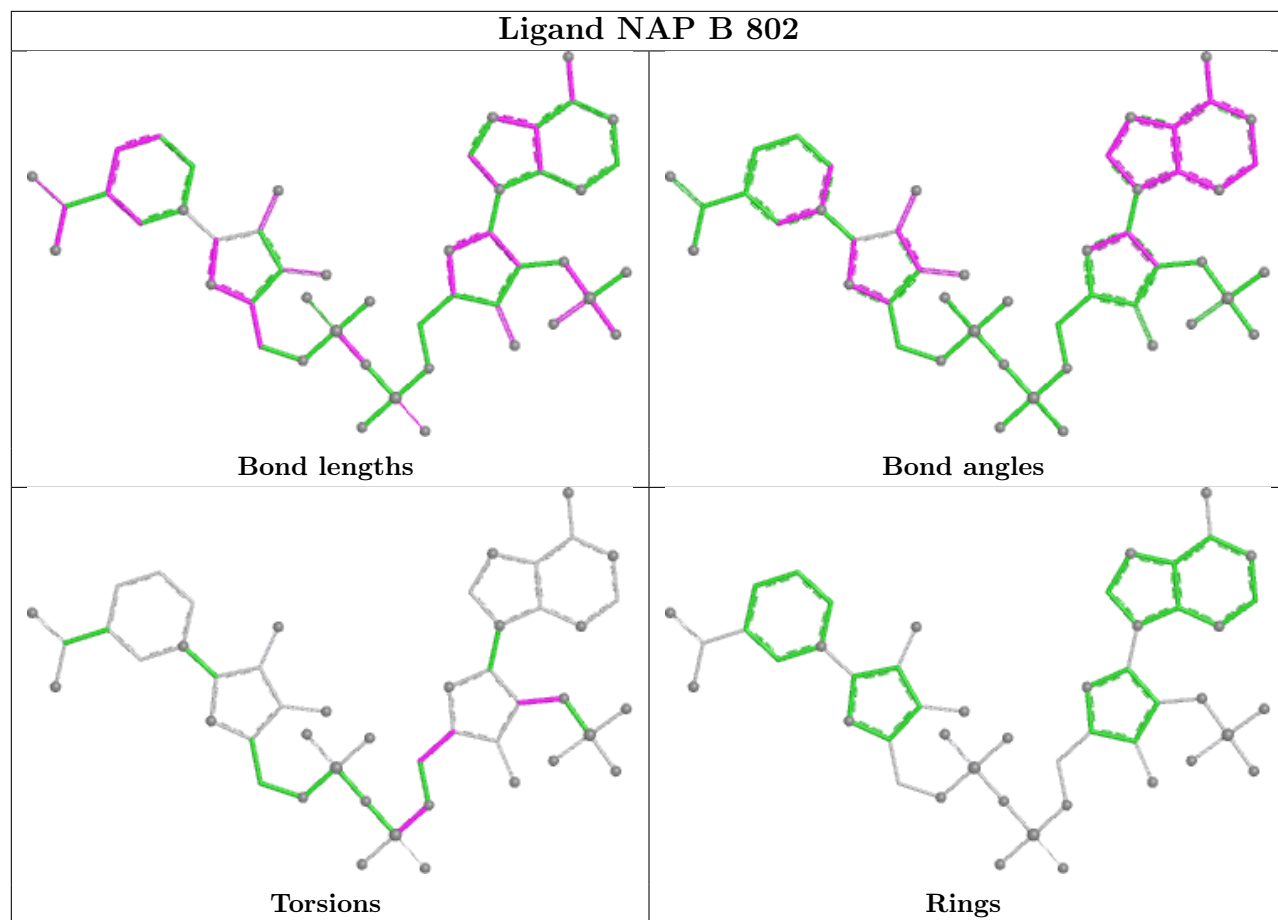
Mol	Chain	Res	Type	Atoms
3	A	802	NAP	C3B-C4B-C5B-O5B
3	A	802	NAP	C1B-C2B-O2B-P2B
3	B	802	NAP	C1B-C2B-O2B-P2B
3	A	802	NAP	O4B-C4B-C5B-O5B
3	B	802	NAP	C5B-O5B-PA-O1A
3	A	802	NAP	C2B-O2B-P2B-O3X
3	A	802	NAP	O4D-C1D-N1N-C2N

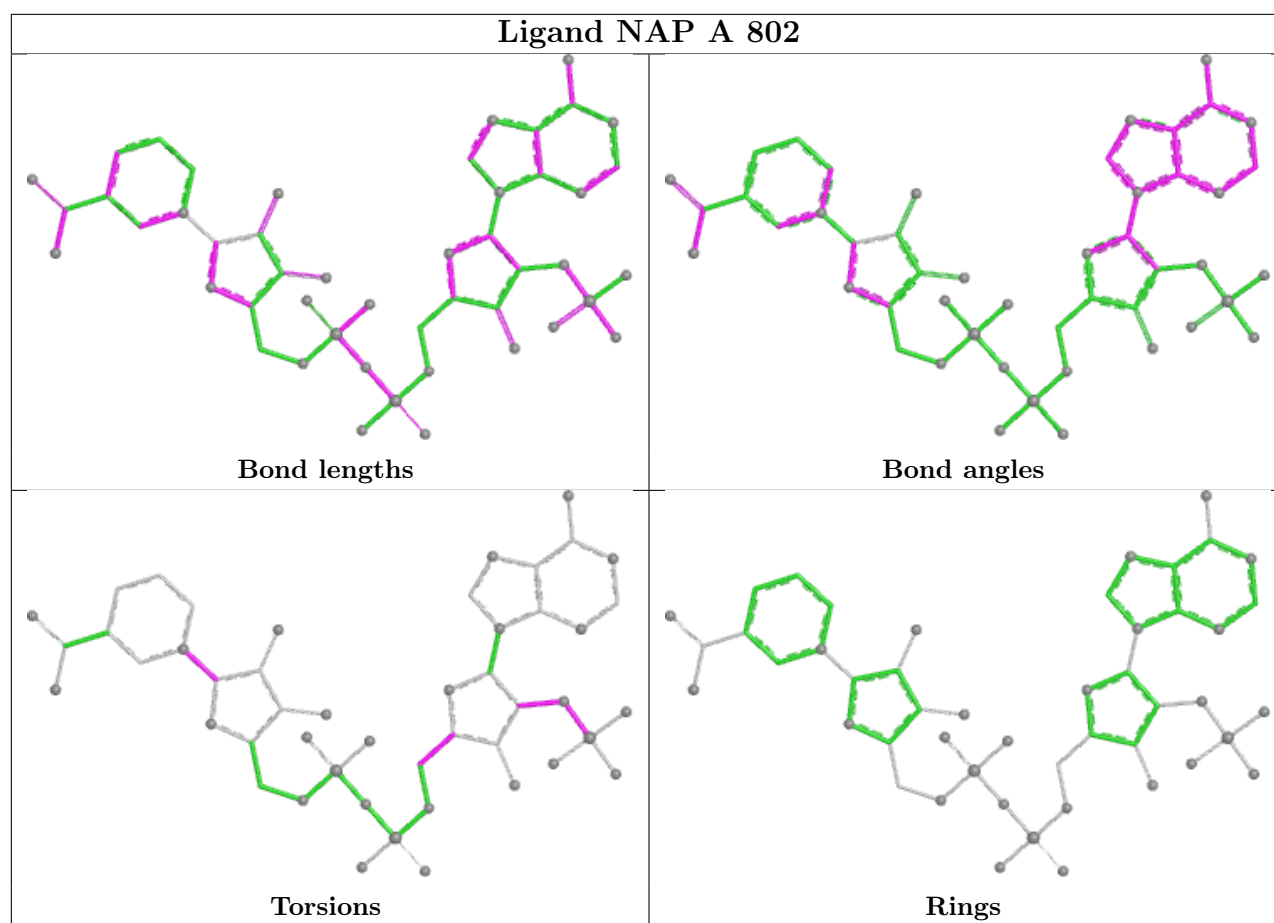
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	NAP	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	405/445 (91%)	0.43	30 (7%)	20 26	12, 33, 68, 91	2 (0%)
1	B	411/445 (92%)	0.27	25 (6%)	27 35	11, 25, 60, 86	0
All	All	816/890 (91%)	0.35	55 (6%)	24 30	11, 29, 64, 91	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	THR	6.3
1	B	425	TRP	4.7
1	A	16	THR	4.5
1	A	296	PHE	4.0
1	A	371	VAL	3.7
1	B	301	PRO	3.5
1	B	278	ALA	3.5
1	B	281	LEU	3.5
1	B	16	THR	3.3
1	B	282	THR	3.2
1	A	384	PHE	3.1
1	B	279	GLY	3.0
1	B	286	LEU	2.9
1	B	277	VAL	2.8
1	B	241	GLY	2.8
1	A	277	VAL	2.8
1	B	306	THR	2.7
1	A	235	GLN	2.7
1	B	283	PRO	2.7
1	A	278	ALA	2.7
1	A	252	TYR	2.6
1	B	252	TYR	2.6
1	B	424	ASP	2.6
1	A	377	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	374	LYS	2.6
1	B	201	VAL	2.5
1	A	315	PRO	2.4
1	A	381	GLY	2.4
1	B	296	PHE	2.4
1	A	305	ILE	2.4
1	B	240	LYS	2.4
1	A	202	ARG	2.4
1	A	201	VAL	2.4
1	B	287	LYS	2.3
1	A	283	PRO	2.3
1	A	243	THR	2.3
1	B	312	ALA	2.3
1	A	253	PHE	2.3
1	B	239	TYR	2.3
1	A	319	ILE	2.3
1	A	306	THR	2.3
1	B	305	ILE	2.3
1	A	379	TYR	2.2
1	A	378	THR	2.2
1	A	17	ASN	2.2
1	A	218	ILE	2.2
1	B	253	PHE	2.1
1	A	380	GLY	2.1
1	B	300	ASN	2.1
1	A	376	SER	2.1
1	B	259	ALA	2.0
1	A	375	VAL	2.0
1	A	309	LYS	2.0
1	A	268	GLY	2.0
1	A	396	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 ⓘ

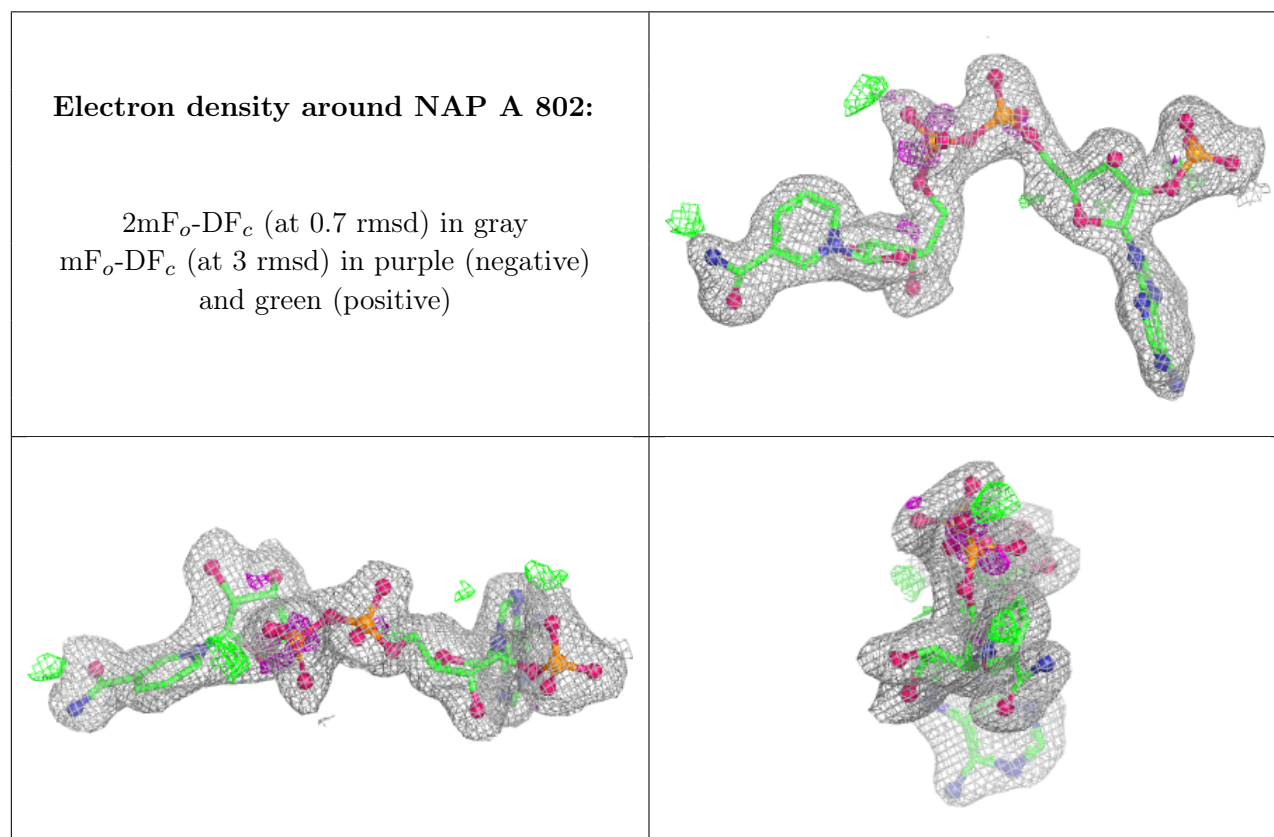
There are no oligosaccharides in this entry.

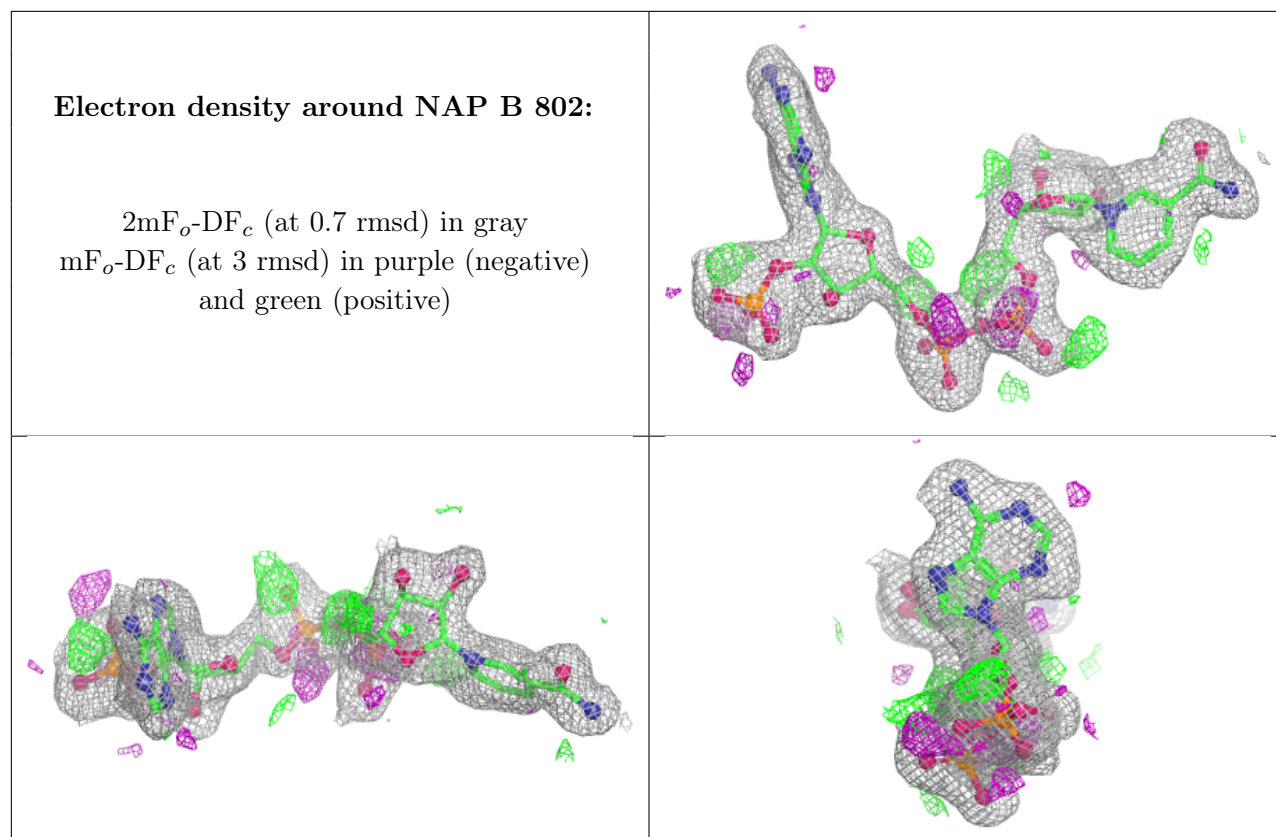
6.4 Ligands [i](#)

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	NAP	A	802	48/48	0.91	0.10	32,44,53,57	0
3	NAP	B	802	48/48	0.91	0.10	27,38,48,61	0
2	MG	A	801	1/1	0.93	0.09	40,40,40,40	0
2	MG	B	801	1/1	0.95	0.13	32,32,32,32	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.