



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:21 PM UTC

PDB ID : 5GZ3 / pdb_00005gz3
Title : Structure of D-amino acid dehydrogenase in complex with NADP
Authors : Sakuraba, H.; Seto, T.; Hayashi, J.; Akita, H.; Yoneda, K.; Ohshima, T.
Deposited on : 2016-09-26
Resolution : 1.59 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

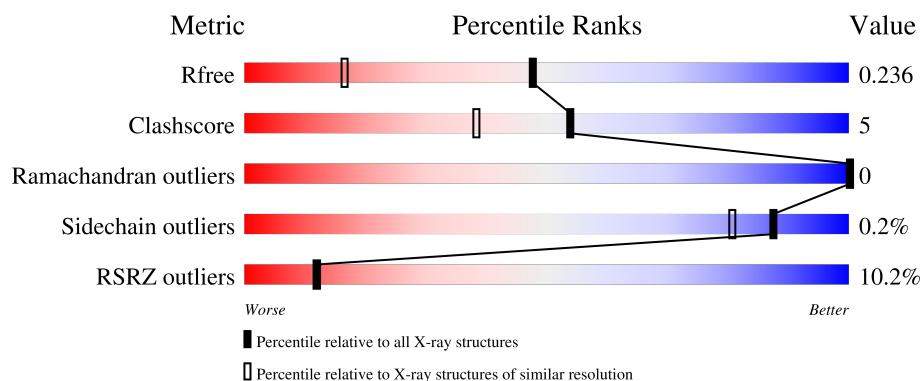
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	326	6% 78% 21%
1	B	326	14% 76% 21% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5465 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 Meso-diaminopimelate D-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2518	1592	433	485	8			
1	B	319	Total	C	N	O	S	0	0	0
			2465	1556	426	476	7			

There are 14 discrepancies between the modelled and reference sequences:

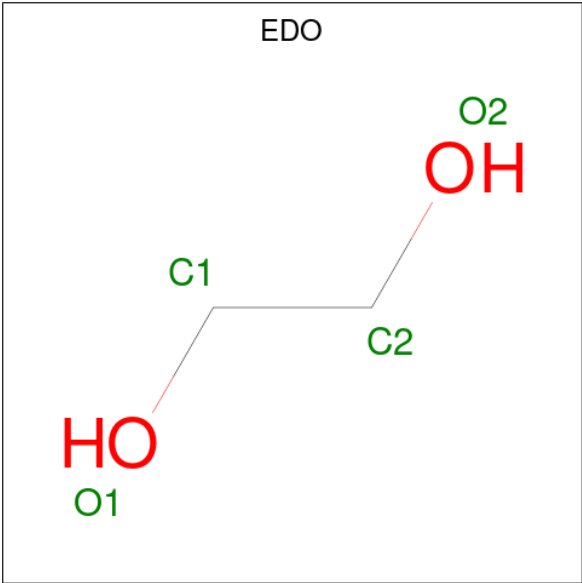
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	ASP	engineered mutation	UNP G1UII1
A	154	LEU	GLN	engineered mutation	UNP G1UII1
A	158	GLY	ASP	engineered mutation	UNP G1UII1
A	173	ILE	THR	engineered mutation	UNP G1UII1
A	199	MET	ARG	engineered mutation	UNP G1UII1
A	224	PHE	TYR	engineered mutation	UNP G1UII1
A	249	ASN	HIS	engineered mutation	UNP G1UII1
B	94	ALA	ASP	engineered mutation	UNP G1UII1
B	154	LEU	GLN	engineered mutation	UNP G1UII1
B	158	GLY	ASP	engineered mutation	UNP G1UII1
B	173	ILE	THR	engineered mutation	UNP G1UII1
B	199	MET	ARG	engineered mutation	UNP G1UII1
B	224	PHE	TYR	engineered mutation	UNP G1UII1
B	249	ASN	HIS	engineered mutation	UNP G1UII1

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

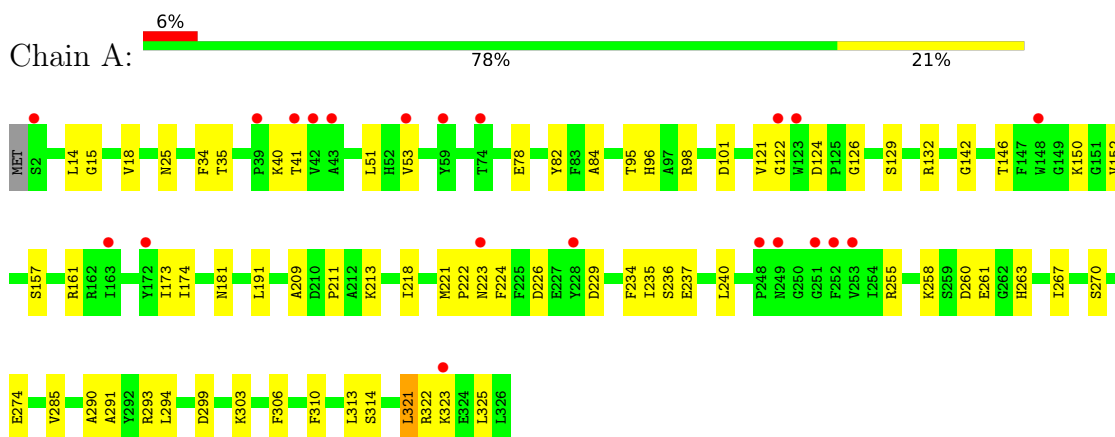
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		
4	B	168	Total	O	0	0
			168	168		

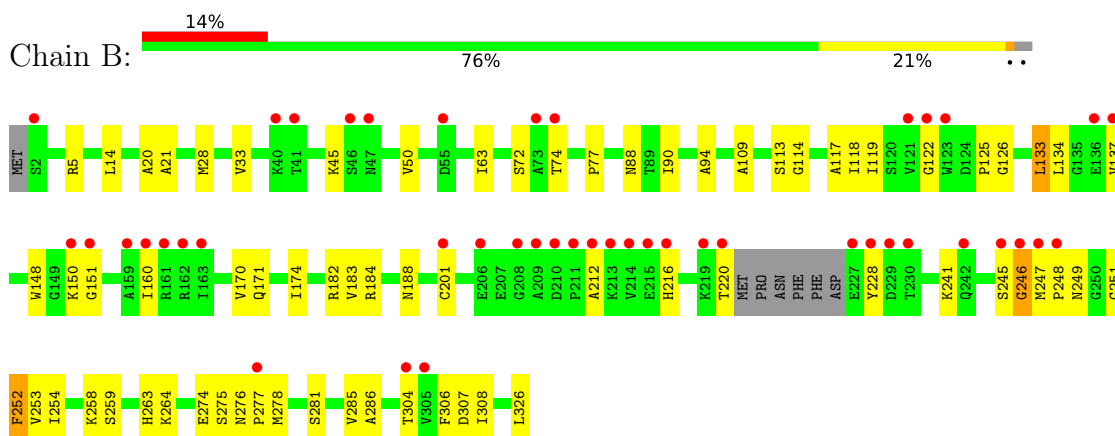
3 Residue-property plots

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: Meso-diaminopimelate D-dehydrogenase



- Molecule 1: Meso-diaminopimelate D-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.59Å 78.23Å 68.97Å 90.00° 107.25° 90.00°	Depositor
Resolution (Å)	50.00 – 1.59 50.00 – 1.59	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-1.59) 93.6 (50.00-1.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.191 , 0.229 0.211 , 0.236	Depositor DCC
R_{free} test set	4073 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5465	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.71	32/2571 (1.2%)	1.44	13/3480 (0.4%)
1	B	1.69	30/2514 (1.2%)	1.42	9/3401 (0.3%)
All	All	1.70	62/5085 (1.2%)	1.43	22/6881 (0.3%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	ASN	C-O	13.03	1.30	1.23
1	B	188	ASN	N-CA	-9.33	1.39	1.46
1	B	254	ILE	CA-CB	-8.53	1.44	1.54
1	A	124	ASP	N-CA	-7.29	1.40	1.46
1	A	132	ARG	C-O	-7.11	1.16	1.24
1	B	90	ILE	C-O	7.09	1.31	1.24
1	B	212	ALA	C-O	-7.02	1.16	1.24
1	A	95	THR	CA-CB	-6.85	1.44	1.52
1	A	152	VAL	CA-CB	6.59	1.62	1.54
1	A	174	ILE	CA-CB	6.51	1.59	1.54
1	A	218	ILE	C-O	6.40	1.31	1.24
1	A	236	SER	N-CA	6.31	1.53	1.45
1	B	88	ASN	N-CA	6.26	1.53	1.46
1	A	82	TYR	N-CA	-6.19	1.39	1.46
1	B	251	GLY	N-CA	6.14	1.50	1.45
1	B	183	VAL	N-CA	-6.13	1.39	1.46
1	B	286	ALA	CA-C	6.13	1.60	1.52
1	A	35	THR	CA-C	6.12	1.60	1.52
1	B	182	ARG	N-CA	6.08	1.53	1.46
1	A	146	THR	N-CA	-6.05	1.38	1.46
1	A	221	MET	C-O	-6.01	1.16	1.24
1	B	63	ILE	N-CA	5.99	1.53	1.46
1	A	121	VAL	CA-C	-5.97	1.45	1.52
1	A	299	ASP	C-O	-5.95	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	ALA	C-O	-5.93	1.16	1.24
1	A	291	ALA	N-CA	5.91	1.53	1.46
1	B	188	ASN	CA-CB	5.87	1.56	1.52
1	A	255	ARG	CZ-NH2	-5.84	1.25	1.33
1	B	253	VAL	CA-CB	-5.83	1.46	1.54
1	A	234	PHE	C-O	5.79	1.31	1.24
1	B	14	LEU	CA-C	-5.75	1.45	1.52
1	B	33	VAL	CA-C	-5.73	1.45	1.52
1	B	148	TRP	N-CA	-5.65	1.39	1.46
1	B	133	LEU	C-O	-5.60	1.17	1.24
1	B	252	PHE	CA-C	5.60	1.59	1.52
1	B	118	ILE	C-O	5.58	1.30	1.24
1	B	119	ILE	CA-C	5.54	1.58	1.52
1	A	213	LYS	N-CA	-5.53	1.39	1.46
1	B	170	VAL	N-CA	-5.50	1.39	1.46
1	A	53	VAL	N-CA	5.47	1.53	1.46
1	A	321	LEU	CA-C	-5.46	1.45	1.52
1	B	50	VAL	CA-C	-5.44	1.45	1.52
1	B	228	TYR	CA-C	5.43	1.59	1.52
1	A	191	LEU	CA-C	-5.41	1.46	1.52
1	B	183	VAL	CA-CB	5.37	1.60	1.54
1	B	308	ILE	N-CA	-5.32	1.42	1.46
1	A	25	ASN	CA-C	5.29	1.59	1.52
1	A	306	PHE	CA-C	-5.25	1.45	1.52
1	B	274	GLU	N-CA	5.24	1.53	1.46
1	A	313	LEU	N-CA	5.20	1.53	1.46
1	A	294	LEU	CA-C	5.20	1.59	1.52
1	A	314	SER	CA-CB	-5.20	1.45	1.53
1	A	18	VAL	C-O	-5.18	1.18	1.24
1	A	15	GLY	C-O	5.17	1.30	1.23
1	A	303	LYS	CA-C	-5.16	1.46	1.52
1	B	109	ALA	N-CA	5.14	1.52	1.46
1	A	293	ARG	CZ-NH1	5.12	1.40	1.32
1	A	84	ALA	C-O	-5.08	1.17	1.24
1	A	270	SER	CA-C	5.03	1.58	1.52
1	B	307	ASP	C-N	5.02	1.38	1.33
1	A	290	ALA	C-O	-5.01	1.17	1.24
1	B	5	ARG	N-CA	-5.01	1.40	1.46

All (22) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	THR	N-CA-C	11.63	124.03	111.36
1	A	224	PHE	N-CA-C	8.41	120.23	111.14
1	B	281	SER	N-CA-C	7.42	120.24	111.71
1	A	174	ILE	CA-C-N	-7.22	112.34	119.78
1	A	174	ILE	C-N-CA	-7.22	112.34	119.78
1	A	41	THR	N-CA-C	6.83	121.77	113.17
1	A	82	TYR	N-CA-C	5.95	117.43	111.07
1	A	285	VAL	N-CA-C	-5.65	105.02	110.72
1	A	226	ASP	N-CA-C	5.58	118.12	111.71
1	B	246	GLY	N-CA-C	5.57	119.67	112.54
1	B	20	ALA	N-CA-C	-5.45	105.42	111.36
1	A	260	ASP	N-CA-C	-5.45	105.89	112.54
1	B	259	SER	N-CA-C	-5.42	103.54	110.53
1	A	142	GLY	O-C-N	-5.36	118.77	123.92
1	B	306	PHE	CA-C-O	5.35	125.93	119.61
1	A	181	ASN	N-CA-C	5.29	117.79	111.71
1	A	40	LYS	N-CA-C	-5.26	105.66	111.71
1	A	267	ILE	N-CA-C	-5.20	100.83	108.11
1	B	117	ALA	CA-C-N	-5.08	116.52	123.12
1	B	117	ALA	C-N-CA	-5.08	116.52	123.12
1	B	113	SER	N-CA-C	5.04	119.14	112.89
1	A	96	HIS	N-CA-C	5.03	117.41	111.33

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	2518	0	2474	25	0
1	B	2465	0	2429	33	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
3	A	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	6	0	0
4	A	202	0	0	4	0
4	B	168	0	0	2	0
All	All	5465	0	4977	49	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 5.

All (49) 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:122:GLY:O	1:A:126:GLY:HA3	1.59	1.00
1:A:98:ARG:NH1	1:A:101:ASP:OD2	2.20	0.74
1:B:246:GLY:C	1:B:248:PRO:HD3	2.13	0.73
1:B:122:GLY:O	1:B:126:GLY:HA3	1.90	0.71
1:B:246:GLY:C	1:B:248:PRO:CD	2.65	0.70
1:A:222:PRO:O	1:A:223:ASN:HB3	1.95	0.64
1:B:247:MET:N	1:B:248:PRO:CD	2.60	0.64
1:B:220:THR:C	4:B:1193:HOH:O	2.40	0.63
1:A:235:ILE:HD11	1:A:240:LEU:HD13	1.80	0.63
1:A:237:GLU:HG2	4:A:1277:HOH:O	1.98	0.63
1:B:160:ILE:HD11	1:B:171:GLN:OE1	2.02	0.58
1:B:184:ARG:NH2	1:B:252:PHE:CE2	2.74	0.54
1:A:323:LYS:HG3	4:A:1221:HOH:O	2.08	0.54
1:B:247:MET:N	1:B:248:PRO:HD3	2.23	0.54
1:A:261:GLU:OE2	1:B:45:LYS:NZ	2.40	0.52
1:A:122:GLY:O	1:A:126:GLY:CA	2.47	0.51
1:A:310:PHE:HB3	1:B:133:LEU:HD22	1.93	0.51
1:A:322:ARG:HD3	1:B:304:THR:HG21	1.91	0.51
1:B:276:ASN:HB3	1:B:277:PRO:CD	2.41	0.50
1:B:72:SER:O	1:B:77:PRO:HD3	2.12	0.49
1:B:275:SER:HB3	1:B:278:MET:HB2	1.96	0.48
1:B:151:GLY:HA3	1:B:249:ASN:HA	1.94	0.48
1:B:28:MET:SD	1:B:285:VAL:HG13	2.53	0.48
1:B:246:GLY:C	1:B:248:PRO:HD2	2.39	0.46
1:B:114:GLY:O	4:B:1101:HOH:O	2.20	0.45
1:A:258:LYS:HA	1:A:263:HIS:O	2.16	0.45
1:B:133:LEU:C	1:B:133:LEU:HD23	2.41	0.45
1:A:322:ARG:CD	1:B:304:THR:HG21	2.47	0.45
1:A:150:LYS:HA	1:A:173:ILE:O	2.16	0.45
1:B:216:HIS:CE1	1:B:220:THR:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:OD2	4:A:1101:HOH:O	2.21	0.43
1:A:274:GLU:HG3	1:B:264:LYS:O	2.18	0.43
1:A:321:LEU:HD22	1:A:325:LEU:HD12	2.00	0.43
1:A:322:ARG:HD3	1:B:304:THR:CG2	2.48	0.43
1:A:263:HIS:CG	1:B:275:SER:HB2	2.53	0.43
1:A:14:LEU:HD11	2:A:1001:NAP:O4D	2.18	0.43
1:B:134:LEU:HA	1:B:137:VAL:HG22	2.01	0.43
1:A:129:SER:HB3	1:B:326:LEU:HA	2.00	0.42
1:B:276:ASN:N	1:B:277:PRO:HD2	2.33	0.42
1:B:150:LYS:HG3	1:B:174:ILE:HG12	2.02	0.42
1:B:94:ALA:HA	1:B:125:PRO:CD	2.50	0.42
1:A:263:HIS:CD2	1:B:275:SER:HB2	2.55	0.41
1:A:323:LYS:NZ	4:A:1111:HOH:O	2.53	0.41
1:B:241:LYS:O	1:B:245:SER:OG	2.36	0.41
1:B:258:LYS:HA	1:B:263:HIS:O	2.21	0.41
1:A:209:ALA:O	1:A:211:PRO:HD3	2.20	0.41
1:B:160:ILE:HD11	1:B:201:CYS:HG	1.85	0.41
1:A:157:SER:O	1:A:161:ARG:HG3	2.21	0.40
1:A:34:PHE:HA	1:A:51:LEU:O	2.21	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	323/326 (99%)	315 (98%)	8 (2%)	0	100	100
1	B	315/326 (97%)	311 (99%)	4 (1%)	0	100	100
All	All	638/652 (98%)	626 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	271/272 (100%)	270 (100%)	1 (0%)	84	75
1	B	265/272 (97%)	265 (100%)	0	100	100
All	All	536/544 (98%)	535 (100%)	1 (0%)	87	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU

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	24	GLN
1	A	57	GLN
1	A	85	GLN
1	B	24	GLN
1	B	57	GLN
1	B	85	GLN
1	B	143	ASN
1	B	188	ASN
1	B	216	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	EDO	A	1003	-	3,3,3	0.65	0	2,2,2	0.17	0
2	NAP	B	1001	-	50,52,52	2.01	9 (18%)	71,80,80	1.72	13 (18%)
3	EDO	B	1002	-	3,3,3	0.44	0	2,2,2	0.71	0
3	EDO	A	1002	-	3,3,3	0.52	0	2,2,2	0.58	0
2	NAP	A	1001	-	50,52,52	1.74	9 (18%)	71,80,80	1.43	10 (14%)
3	EDO	A	1004	-	3,3,3	0.50	0	2,2,2	0.23	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	EDO	A	1003	-	-	0/1/1/1	-
2	NAP	B	1001	-	-	0/35/67/67	0/5/5/5
3	EDO	B	1002	-	-	0/1/1/1	-
3	EDO	A	1002	-	-	0/1/1/1	-
2	NAP	A	1001	-	-	1/35/67/67	0/5/5/5
3	EDO	A	1004	-	-	0/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAP	PN-O3	7.35	1.67	1.59
2	B	1001	NAP	P2B-O2B	7.32	1.72	1.59
2	A	1001	NAP	C5A-C4A	5.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	NAP	PN-O3	5.14	1.65	1.59
2	B	1001	NAP	C5A-C4A	5.02	1.48	1.39
2	B	1001	NAP	P2B-O2X	-4.06	1.39	1.54
2	B	1001	NAP	C2N-N1N	3.71	1.39	1.35
2	A	1001	NAP	C2N-N1N	3.42	1.38	1.35
2	B	1001	NAP	PA-O3	3.39	1.63	1.59
2	B	1001	NAP	O4B-C4B	-3.30	1.37	1.45
2	A	1001	NAP	C5A-C6A	2.82	1.48	1.41
2	A	1001	NAP	PA-O3	2.62	1.62	1.59
2	A	1001	NAP	C4A-N9A	-2.37	1.32	1.37
2	B	1001	NAP	C5A-C6A	2.37	1.47	1.41
2	A	1001	NAP	P2B-O2X	-2.36	1.46	1.54
2	B	1001	NAP	C8A-N7A	2.30	1.36	1.31
2	A	1001	NAP	P2B-O2B	2.15	1.63	1.59
2	A	1001	NAP	C8A-N7A	2.13	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	NAP	C4D-O4D-C1D	-5.78	104.63	109.92
2	A	1001	NAP	C5A-C4A-N3A	-4.39	120.67	126.72
2	B	1001	NAP	P2B-O2B-C2B	-4.36	111.78	123.43
2	B	1001	NAP	C5A-C4A-N3A	-4.09	121.08	126.72
2	B	1001	NAP	N3A-C2A-N1A	-3.97	122.57	128.58
2	A	1001	NAP	C4D-O4D-C1D	-3.77	106.47	109.92
2	B	1001	NAP	O3X-P2B-O2X	3.73	121.78	107.80
2	B	1001	NAP	N3A-C4A-N9A	3.41	132.97	127.17
2	A	1001	NAP	N3A-C4A-N9A	3.33	132.83	127.17
2	B	1001	NAP	C2A-N3A-C4A	3.06	119.31	111.83
2	A	1001	NAP	O2N-PN-O1N	3.06	126.67	112.44
2	B	1001	NAP	O2A-PA-O3	-3.00	99.17	107.27
2	B	1001	NAP	C2A-N1A-C6A	2.92	123.52	118.73
2	A	1001	NAP	N3A-C2A-N1A	-2.90	124.20	128.58
2	A	1001	NAP	C2A-N3A-C4A	2.87	118.85	111.83
2	A	1001	NAP	C4A-C5A-N7A	-2.76	107.42	110.58
2	A	1001	NAP	C2A-N1A-C6A	2.60	123.00	118.73
2	B	1001	NAP	O2B-C2B-C1B	2.50	118.84	110.05
2	A	1001	NAP	C2B-C1B-N9A	-2.38	109.83	113.75
2	B	1001	NAP	C3N-C7N-N7N	2.36	120.65	117.74
2	B	1001	NAP	O2B-P2B-O1X	-2.25	101.32	109.33
2	B	1001	NAP	C4A-C5A-N7A	-2.05	108.24	110.58
2	A	1001	NAP	C6A-C5A-N7A	2.03	136.00	132.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

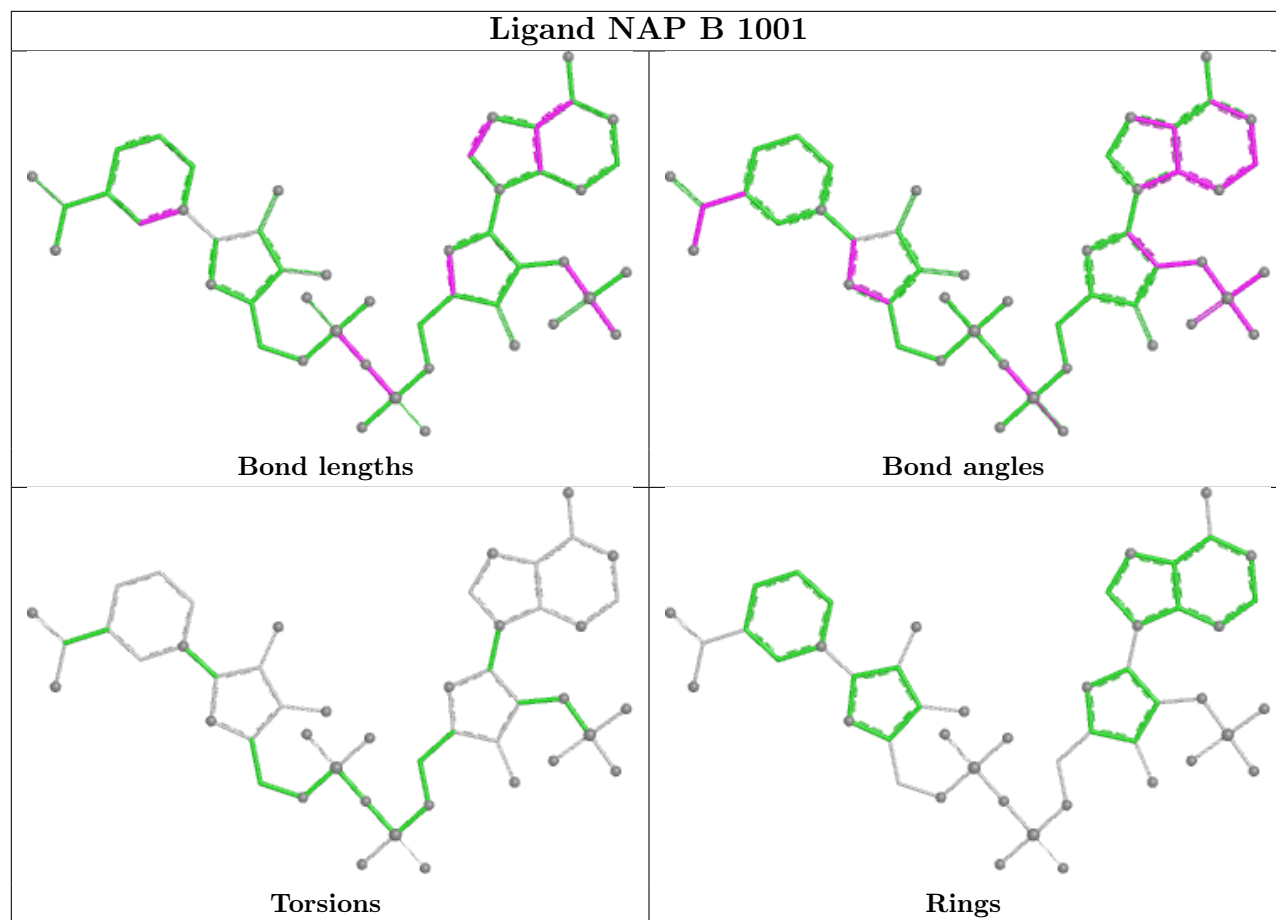
Mol	Chain	Res	Type	Atoms
2	A	1001	NAP	C2B-O2B-P2B-O3X

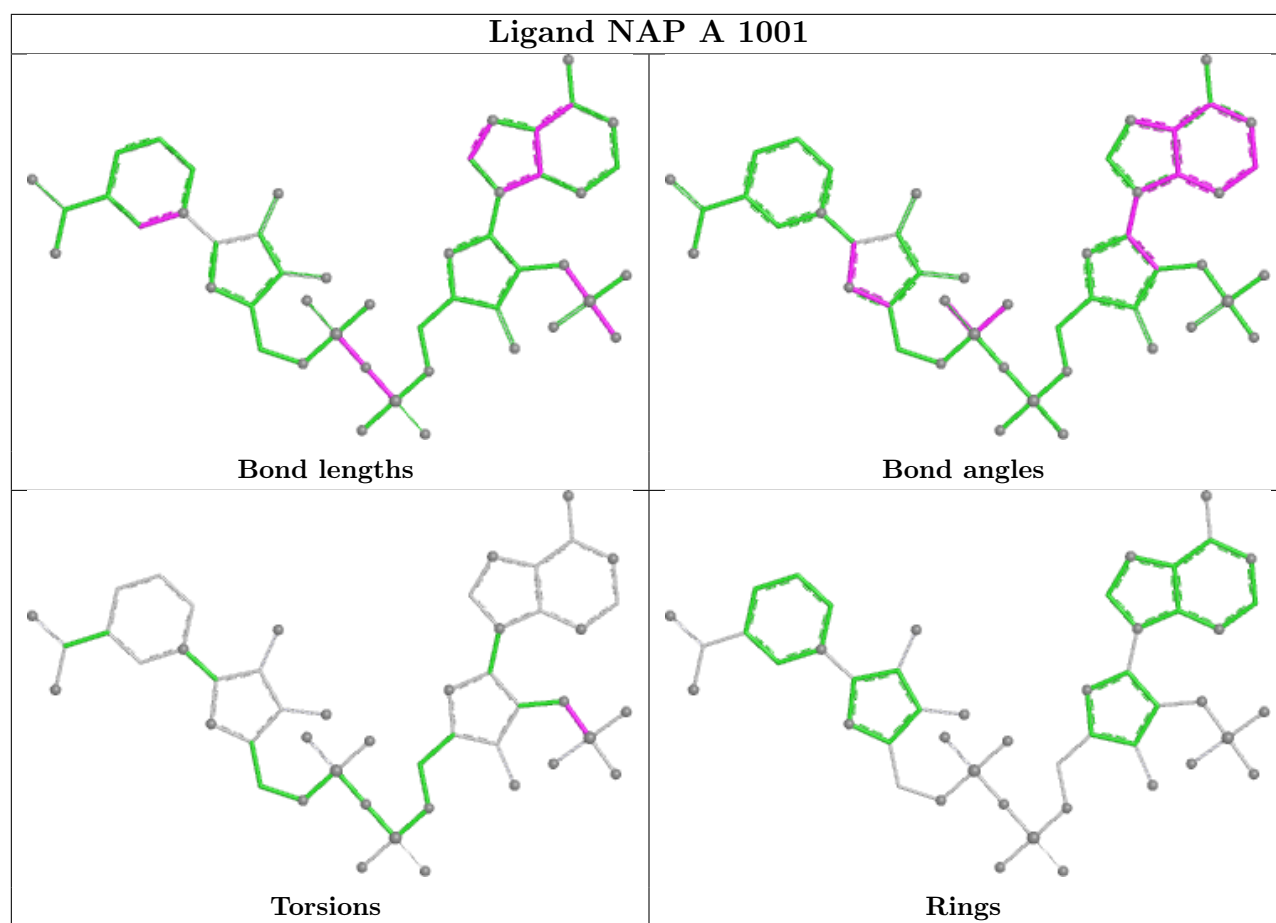
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	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	325/326 (99%)	0.65	21 (6%) 25 25	12, 18, 32, 48	0
1	B	319/326 (97%)	0.87	45 (14%) 6 6	11, 19, 39, 54	0
All	All	644/652 (98%)	0.76	66 (10%) 12 12	11, 18, 36, 54	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	9.9
1	A	122	GLY	6.0
1	B	122	GLY	5.3
1	B	208	GLY	4.7
1	B	212	ALA	4.6
1	B	123	TRP	4.3
1	B	220	THR	4.1
1	B	230	THR	4.0
1	B	209	ALA	3.9
1	A	253	VAL	3.7
1	B	163	ILE	3.7
1	B	73	ALA	3.6
1	B	304	THR	3.5
1	A	223	ASN	3.4
1	B	160	ILE	3.4
1	B	216	HIS	3.3
1	B	228	TYR	3.3
1	A	2	SER	3.2
1	A	252	PHE	3.2
1	A	41	THR	3.2
1	B	248	PRO	3.2
1	B	137	VAL	3.1
1	B	245	SER	3.1
1	B	211	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	TRP	3.0
1	B	214	VAL	2.9
1	A	228	TYR	2.9
1	B	159	ALA	2.8
1	B	305	VAL	2.8
1	B	47	ASN	2.8
1	B	227	GLU	2.8
1	B	219	LYS	2.8
1	B	247	MET	2.8
1	B	201	CYS	2.7
1	A	172	TYR	2.6
1	B	151	GLY	2.6
1	B	121	VAL	2.6
1	A	148	TRP	2.6
1	A	43	ALA	2.6
1	B	206	GLU	2.6
1	B	161	ARG	2.5
1	B	210	ASP	2.5
1	B	74	THR	2.5
1	B	150	LYS	2.4
1	B	2	SER	2.4
1	B	229	ASP	2.4
1	B	46	SER	2.4
1	A	323	LYS	2.3
1	B	213	LYS	2.3
1	A	53	VAL	2.3
1	A	42	VAL	2.3
1	B	55	ASP	2.3
1	A	249	ASN	2.2
1	A	248	PRO	2.2
1	B	40	LYS	2.2
1	B	41	THR	2.2
1	B	162	ARG	2.1
1	A	74	THR	2.1
1	A	251	GLY	2.1
1	B	242	GLN	2.1
1	A	163	ILE	2.0
1	A	39	PRO	2.0
1	B	277	PRO	2.0
1	B	136	GLU	2.0
1	B	215	GLU	2.0
1	A	59	TYR	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](#)

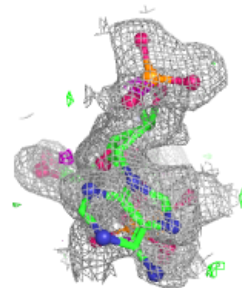
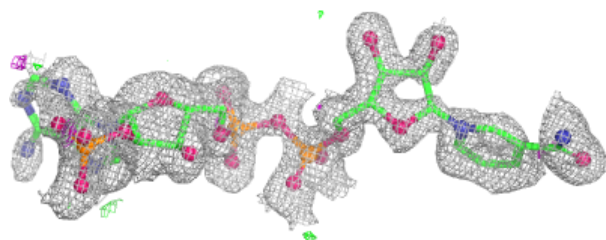
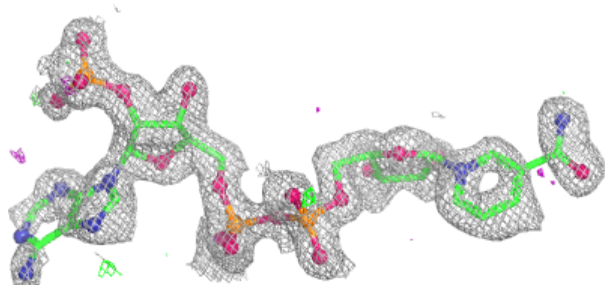
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	1002	4/4	0.93	0.09	19,19,20,21	0
3	EDO	B	1002	4/4	0.93	0.09	19,20,21,24	0
2	NAP	A	1001	48/48	0.94	0.10	18,23,39,45	0
2	NAP	B	1001	48/48	0.95	0.09	14,18,33,36	0
3	EDO	A	1004	4/4	0.97	0.05	13,13,14,15	0
3	EDO	A	1003	4/4	0.97	0.06	22,24,24,26	0

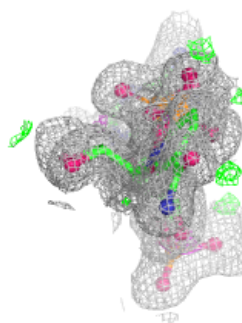
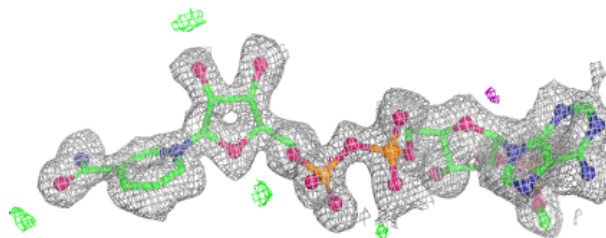
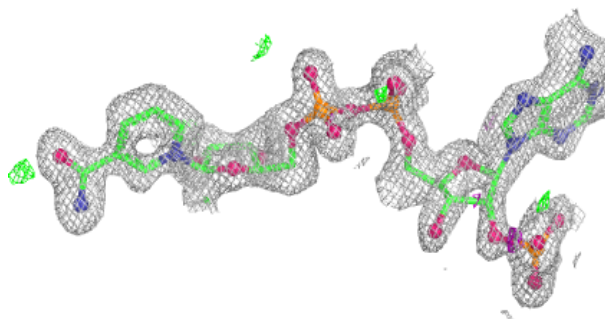
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP A 1001:

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

**Electron density around NAP B 1001:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.