



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:37 AM UTC

PDB ID : 3WYC / pdb_00003wyc
Title : Structure of a meso-diaminopimelate dehydrogenase in complex with NADP
Authors : Sakuraba, H.; Akita, H.; Ohshima, T.
Deposited on : 2014-08-25
Resolution : 2.07 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

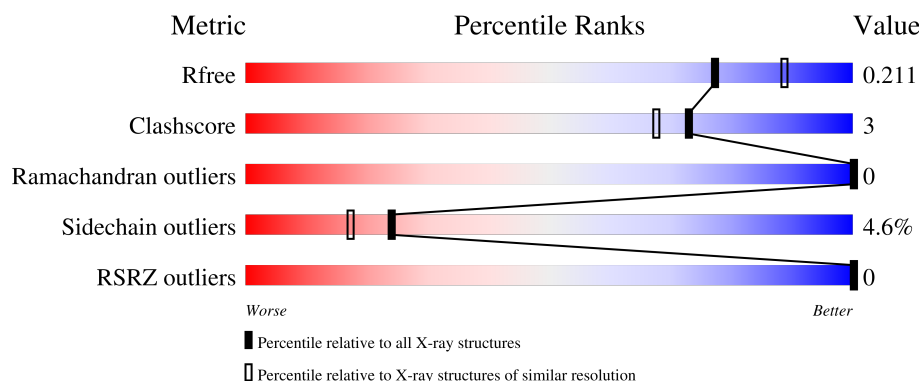
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	334	
1	B	334	

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	NES	A	1003	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5623 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	327	Total	C	N	O	S	0	0	0
			2542	1602	440	493	7			
1	B	327	Total	C	N	O	S	0	0	0
			2542	1602	440	493	7			

There are 16 discrepancies between the modelled and reference sequences:

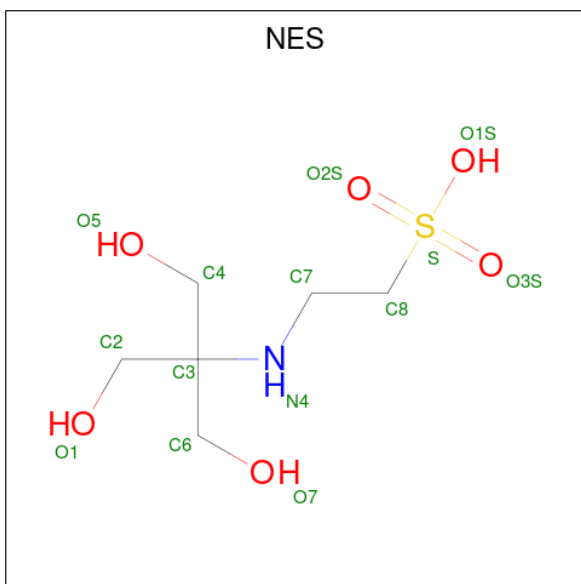
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	THR	-	expression tag	UNP G1UII1
A	328	ARG	-	expression tag	UNP G1UII1
A	329	HIS	-	expression tag	UNP G1UII1
A	330	HIS	-	expression tag	UNP G1UII1
A	331	HIS	-	expression tag	UNP G1UII1
A	332	HIS	-	expression tag	UNP G1UII1
A	333	HIS	-	expression tag	UNP G1UII1
A	334	HIS	-	expression tag	UNP G1UII1
B	327	THR	-	expression tag	UNP G1UII1
B	328	ARG	-	expression tag	UNP G1UII1
B	329	HIS	-	expression tag	UNP G1UII1
B	330	HIS	-	expression tag	UNP G1UII1
B	331	HIS	-	expression tag	UNP G1UII1
B	332	HIS	-	expression tag	UNP G1UII1
B	333	HIS	-	expression tag	UNP G1UII1
B	334	HIS	-	expression tag	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 2-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-ETHANESULFONIC ACID (CCD ID: NES) (formula: $\text{C}_6\text{H}_{15}\text{NO}_6\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	6	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	6	1	6	1		
3	B	1	Total	C	N	O	S	0	0
			14	6	1	6	1		
3	B	1	Total	C	N	O	S	0	0
			14	6	1	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	193	Total	O	0	0
			193	193		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	123.02Å 123.02Å 193.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.12 – 2.07 31.12 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.12-2.07) 99.8 (31.12-2.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.97 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.173 , 0.208 0.186 , 0.211	Depositor DCC
R_{free} test set	3365 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5623	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 5.14% 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: NES, 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	1.50	22/2596 (0.8%)	1.19	9/3517 (0.3%)
1	B	1.48	17/2596 (0.7%)	1.20	6/3517 (0.2%)
All	All	1.49	39/5192 (0.8%)	1.20	15/7034 (0.2%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	ASN	C-O	-8.02	1.16	1.24
1	B	56	ALA	N-CA	7.20	1.54	1.46
1	A	276	ASN	C-O	-7.16	1.17	1.24
1	A	188	ASN	C-O	6.62	1.26	1.23
1	A	161	ARG	C-O	-6.23	1.16	1.24
1	B	108	ALA	N-CA	6.18	1.53	1.46
1	A	139	LEU	C-N	6.09	1.41	1.33
1	B	307	ASP	CA-C	-6.05	1.44	1.52
1	B	274	GLU	C-O	-6.04	1.17	1.24
1	A	166	VAL	C-O	-5.91	1.17	1.24
1	A	154	GLN	C-O	-5.86	1.17	1.24
1	A	221	MET	CA-C	5.77	1.59	1.52
1	B	139	LEU	C-N	5.73	1.40	1.33
1	A	311	GLY	CA-C	5.68	1.58	1.52
1	A	274	GLU	C-O	-5.67	1.17	1.24
1	B	276	ASN	C-N	5.60	1.41	1.34
1	A	42	VAL	N-CA	5.57	1.53	1.46
1	A	102	TYR	C-O	5.56	1.30	1.24
1	A	276	ASN	C-N	5.56	1.41	1.34
1	A	138	VAL	C-O	-5.52	1.17	1.24
1	A	56	ALA	N-CA	5.51	1.52	1.46
1	A	170	VAL	C-O	-5.48	1.18	1.24
1	A	167	LYS	C-O	-5.44	1.17	1.24
1	B	104	ASP	N-CA	5.43	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	THR	CA-C	-5.35	1.46	1.52
1	B	138	VAL	C-O	-5.29	1.17	1.24
1	B	154	GLN	C-O	-5.27	1.18	1.24
1	B	248	PRO	N-CD	5.27	1.55	1.47
1	A	108	ALA	N-CA	5.22	1.52	1.46
1	B	176	ILE	CA-C	5.21	1.58	1.52
1	B	4	ILE	CA-C	5.19	1.58	1.52
1	A	249	HIS	C-O	-5.18	1.18	1.24
1	A	104	ASP	N-CA	5.10	1.52	1.46
1	B	140	PRO	N-CD	5.06	1.54	1.47
1	A	277	PRO	N-CD	5.05	1.54	1.47
1	A	324	GLU	CA-C	5.02	1.59	1.52
1	B	42	VAL	N-CA	5.02	1.52	1.46
1	A	14	LEU	C-O	-5.01	1.18	1.24
1	B	311	GLY	CA-C	5.01	1.58	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LYS	N-CA-C	9.61	121.84	111.36
1	A	38	ASP	CA-C-N	6.16	126.62	119.47
1	A	38	ASP	C-N-CA	6.16	126.62	119.47
1	B	38	ASP	CA-C-N	5.73	126.12	119.47
1	B	38	ASP	C-N-CA	5.73	126.12	119.47
1	A	167	LYS	N-CA-C	5.72	117.31	111.14
1	A	245	SER	N-CA-C	5.51	119.72	112.89
1	B	245	SER	N-CA-C	5.36	119.66	113.18
1	B	139	LEU	CA-C-N	-5.31	114.15	119.56
1	B	139	LEU	C-N-CA	-5.31	114.15	119.56
1	A	190	GLU	N-CA-C	-5.27	100.58	108.96
1	B	138	VAL	N-CA-C	5.22	115.99	110.72
1	A	139	LEU	CA-C-N	-5.08	114.38	119.56
1	A	139	LEU	C-N-CA	-5.08	114.38	119.56
1	A	195	GLU	N-CA-C	5.08	116.90	111.36

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	2542	0	2481	24	0
1	B	2542	0	2481	21	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
3	A	28	0	30	1	0
3	B	28	0	30	0	0
4	A	194	0	0	2	0
4	B	193	0	0	0	0
All	All	5623	0	5072	33	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 3.

All (33) 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:99:ILE:HD12	1:B:327:THR:HG21	1.30	1.07
1:A:99:ILE:CD1	1:B:327:THR:HG21	1.91	1.00
1:A:99:ILE:CD1	1:B:327:THR:CG2	2.41	0.98
1:A:99:ILE:HD12	1:B:327:THR:CG2	1.94	0.96
1:A:99:ILE:CD1	1:B:327:THR:HG22	2.11	0.78
1:A:162:ARG:HD3	4:A:1252:HOH:O	1.84	0.77
1:A:99:ILE:HD13	1:B:327:THR:HG22	1.71	0.71
1:A:233:HIS:HD2	4:A:1235:HOH:O	1.74	0.68
1:A:327:THR:HG22	1:B:99:ILE:CD1	2.30	0.61
1:A:327:THR:OG1	1:A:328:ARG:N	2.40	0.54
1:A:327:THR:HG21	1:B:96:HIS:HA	1.89	0.54
1:B:192:SER:OG	1:B:195:GLU:HG3	2.07	0.53
1:A:184:ARG:NH2	1:A:252:PHE:CE1	2.78	0.52
1:B:184:ARG:NH2	1:B:252:PHE:CE1	2.80	0.50
1:A:96:HIS:HA	1:B:327:THR:HG21	1.94	0.50
1:A:98:ARG:NH2	1:A:101:ASP:OD2	2.45	0.49
1:A:46:SER:O	1:A:47:ASN:C	2.55	0.49
1:A:247:MET:N	1:A:248:PRO:CD	2.75	0.49
1:A:327:THR:CG2	1:B:99:ILE:CD1	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:THR:CG2	1:B:99:ILE:HD12	2.43	0.48
1:B:222:PRO:O	1:B:223:ASN:HB2	2.13	0.47
3:A:1003:NES:O3S	3:A:1003:NES:N4	2.48	0.47
1:A:96:HIS:HA	1:B:327:THR:CG2	2.46	0.45
1:A:221:MET:HA	1:A:222:PRO:HD3	1.86	0.45
1:A:327:THR:CG2	1:B:96:HIS:HA	2.47	0.44
1:A:246:GLY:C	1:A:248:PRO:CD	2.91	0.44
1:B:221:MET:HA	1:B:222:PRO:HD3	1.86	0.43
1:A:222:PRO:O	1:A:223:ASN:HB2	2.19	0.42
1:B:151:GLY:HA3	1:B:249:HIS:HA	2.00	0.42
1:B:9:VAL:HG23	1:B:66:MET:HG3	2.02	0.42
1:B:108:ALA:O	1:B:112:GLN:HB2	2.20	0.42
1:A:151:GLY:HA3	1:A:249:HIS:HA	2.02	0.41
1:B:167:LYS:O	1:B:167:LYS:HG2	2.22	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	325/334 (97%)	319 (98%)	6 (2%)	0	100	100
1	B	325/334 (97%)	320 (98%)	5 (2%)	0	100	100
All	All	650/668 (97%)	639 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	274/282 (97%)	260 (95%)	14 (5%)	21	14
1	B	274/282 (97%)	263 (96%)	11 (4%)	28	22
All	All	548/564 (97%)	523 (95%)	25 (5%)	24	17

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	99	ILE
1	A	134	LEU
1	A	171	GLN
1	A	196	LYS
1	A	249	HIS
1	A	264	LYS
1	A	265	GLN
1	A	266	ILE
1	A	276	ASN
1	A	294	LEU
1	A	295	SER
1	A	326	LEU
1	A	327	THR
1	B	99	ILE
1	B	112	GLN
1	B	134	LEU
1	B	164	GLN
1	B	171	GLN
1	B	249	HIS
1	B	276	ASN
1	B	294	LEU
1	B	300	LYS
1	B	326	LEU
1	B	327	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	96	HIS
1	A	164	GLN
1	A	223	ASN
1	A	233	HIS
1	B	57	GLN
1	B	85	GLN
1	B	223	ASN
1	B	243	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	NES	A	1002	-	13,13,13	1.65	3 (23%)	17,18,18	2.63	9 (52%)
2	NAP	B	1001	-	50,52,52	1.93	17 (34%)	71,80,80	1.51	11 (15%)
3	NES	B	1003	-	13,13,13	2.66	3 (23%)	17,18,18	2.35	5 (29%)
3	NES	B	1002	-	13,13,13	1.53	2 (15%)	17,18,18	2.66	8 (47%)
3	NES	A	1003	-	13,13,13	2.62	4 (30%)	17,18,18	3.10	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	1001	-	50,52,52	1.92	17 (34%)	71,80,80	1.59	13 (18%)

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	NES	A	1002	-	-	3/17/17/17	-
2	NAP	B	1001	-	-	0/35/67/67	0/5/5/5
3	NES	B	1003	-	-	6/17/17/17	-
3	NES	B	1002	-	-	0/17/17/17	-
3	NES	A	1003	-	-	11/17/17/17	-
2	NAP	A	1001	-	-	0/35/67/67	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	NES	C8-S	-6.93	1.67	1.77
3	B	1003	NES	C8-S	-6.70	1.68	1.77
3	B	1003	NES	O1S-S	5.35	1.67	1.47
3	A	1003	NES	O1S-S	5.12	1.66	1.47
2	B	1001	NAP	C5A-N7A	-4.62	1.30	1.39
2	A	1001	NAP	C5A-N7A	-4.45	1.31	1.39
2	A	1001	NAP	PA-O3	-3.96	1.55	1.59
2	B	1001	NAP	PA-O3	-3.94	1.55	1.59
3	A	1002	NES	O1S-S	3.91	1.61	1.47
3	B	1002	NES	O1S-S	3.83	1.61	1.47
2	A	1001	NAP	C5A-C4A	3.70	1.45	1.39
2	A	1001	NAP	P2B-O2X	-3.56	1.41	1.54
2	B	1001	NAP	C5A-C4A	3.50	1.45	1.39
2	A	1001	NAP	O7N-C7N	-3.32	1.17	1.24
2	A	1001	NAP	C4A-N9A	-3.28	1.30	1.37
2	B	1001	NAP	C4A-N9A	-3.24	1.30	1.37
2	A	1001	NAP	P2B-O3X	-3.18	1.43	1.54
2	B	1001	NAP	P2B-O2X	-3.13	1.43	1.54
2	B	1001	NAP	P2B-O3X	-3.12	1.43	1.54
2	B	1001	NAP	PN-O2N	-3.11	1.40	1.55
2	A	1001	NAP	C2N-N1N	-3.07	1.31	1.35
2	B	1001	NAP	C2N-N1N	-3.07	1.31	1.35
2	B	1001	NAP	O7N-C7N	-3.00	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1003	NES	C6-C3	2.91	1.56	1.53
2	B	1001	NAP	PA-O1A	-2.81	1.41	1.50
2	A	1001	NAP	PA-O1A	-2.72	1.41	1.50
3	A	1002	NES	C2-C3	2.68	1.56	1.53
2	A	1001	NAP	PN-O1N	-2.68	1.41	1.50
2	A	1001	NAP	PN-O2N	-2.54	1.43	1.55
2	B	1001	NAP	P2B-O2B	-2.52	1.55	1.59
2	B	1001	NAP	PN-O1N	-2.52	1.42	1.50
2	B	1001	NAP	O4D-C4D	-2.43	1.39	1.45
3	A	1003	NES	C6-C3	-2.34	1.50	1.53
2	A	1001	NAP	O4D-C4D	-2.31	1.39	1.45
3	A	1003	NES	C4-C3	2.31	1.56	1.53
2	B	1001	NAP	PA-O2A	-2.28	1.44	1.55
2	A	1001	NAP	P2B-O2B	-2.26	1.55	1.59
2	A	1001	NAP	C8A-N9A	-2.23	1.33	1.37
2	B	1001	NAP	P2B-O1X	-2.22	1.43	1.50
2	A	1001	NAP	PA-O2A	-2.20	1.45	1.55
2	A	1001	NAP	P2B-O1X	-2.18	1.43	1.50
2	A	1001	NAP	O4B-C4B	-2.16	1.40	1.45
2	B	1001	NAP	C8A-N9A	-2.12	1.33	1.37
3	A	1002	NES	C7-N4	2.10	1.49	1.46
2	B	1001	NAP	O4B-C4B	-2.04	1.40	1.45
3	B	1002	NES	C2-C3	2.02	1.55	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	NES	C7-N4-C3	7.30	126.85	116.17
3	A	1002	NES	C7-N4-C3	6.44	125.58	116.17
3	B	1002	NES	C7-N4-C3	6.27	125.34	116.17
3	B	1003	NES	C7-N4-C3	6.18	125.21	116.17
2	B	1001	NAP	C5A-C4A-N3A	-5.60	119.00	126.72
2	A	1001	NAP	C5A-C4A-N3A	-5.49	119.16	126.72
3	A	1003	NES	C4-C3-C2	5.05	121.09	110.02
2	B	1001	NAP	N3A-C4A-N9A	4.83	135.39	127.17
3	A	1003	NES	O7-C6-C3	-4.82	101.88	111.68
2	A	1001	NAP	N3A-C4A-N9A	4.70	135.17	127.17
3	A	1003	NES	O2S-S-C8	4.44	113.43	106.73
3	A	1002	NES	O1S-S-C8	-4.21	97.77	106.00
3	A	1002	NES	O7-C6-C3	-4.11	103.33	111.68
3	B	1002	NES	O1S-S-C8	-3.78	98.61	106.00
3	B	1002	NES	O7-C6-C3	-3.76	104.04	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	NES	O1S-S-O2S	3.50	120.14	111.40
3	B	1003	NES	O1S-S-O3S	-3.47	102.73	111.40
2	A	1001	NAP	C3N-C7N-N7N	3.44	121.98	117.74
2	B	1001	NAP	C2A-N3A-C4A	3.43	120.20	111.83
3	B	1003	NES	O1-C2-C3	-3.40	104.76	111.68
3	A	1003	NES	C6-C3-C4	-3.32	102.73	110.02
3	B	1003	NES	O1S-S-C8	3.24	112.34	106.00
2	B	1001	NAP	N3A-C2A-N1A	-3.12	123.86	128.58
2	A	1001	NAP	C2A-N3A-C4A	3.02	119.21	111.83
3	B	1002	NES	O1S-S-O3S	2.96	118.79	111.40
3	B	1002	NES	O3S-S-O2S	-2.89	104.44	113.82
2	A	1001	NAP	O7N-C7N-N7N	-2.75	118.65	122.62
3	A	1002	NES	O1S-S-O3S	2.68	118.10	111.40
2	A	1001	NAP	O2N-PN-O1N	2.64	124.73	112.44
2	B	1001	NAP	O7N-C7N-N7N	-2.60	118.86	122.62
3	A	1003	NES	O1S-S-O3S	-2.55	105.02	111.40
2	A	1001	NAP	C4D-O4D-C1D	2.52	112.23	109.92
3	A	1002	NES	O1S-S-O2S	2.51	117.69	111.40
2	A	1001	NAP	O3X-P2B-O2X	2.43	116.90	107.80
2	A	1001	NAP	N3A-C2A-N1A	-2.38	124.98	128.58
3	B	1003	NES	O2S-S-C8	2.37	110.30	106.73
2	A	1001	NAP	C4A-C5A-N7A	-2.34	107.90	110.58
2	A	1001	NAP	N6A-C6A-N1A	2.27	123.44	118.38
2	B	1001	NAP	C2A-N1A-C6A	2.25	122.43	118.73
2	A	1001	NAP	C2A-N1A-C6A	2.24	122.41	118.73
3	A	1003	NES	C6-C3-N4	2.23	115.66	109.02
2	B	1001	NAP	C2B-C1B-N9A	-2.21	110.11	113.75
3	B	1002	NES	O3S-S-C8	-2.20	103.40	106.73
3	A	1002	NES	O2S-S-C8	2.20	110.06	106.73
3	A	1002	NES	O5-C4-C3	-2.18	107.26	111.68
2	A	1001	NAP	O3B-C3B-C2B	2.10	117.08	111.19
3	B	1002	NES	O2S-S-C8	2.09	109.89	106.73
3	A	1002	NES	O3S-S-O2S	-2.06	107.11	113.82
2	B	1001	NAP	C4A-N9A-C8A	2.05	107.89	105.74
2	B	1001	NAP	O2N-PN-O3	-2.04	101.76	107.27
2	B	1001	NAP	C4A-C5A-N7A	-2.02	108.28	110.58
3	A	1002	NES	C8-C7-N4	2.02	117.36	111.41
2	B	1001	NAP	C3N-C7N-N7N	2.00	120.21	117.74
3	A	1003	NES	O3S-S-O2S	-2.00	107.31	113.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

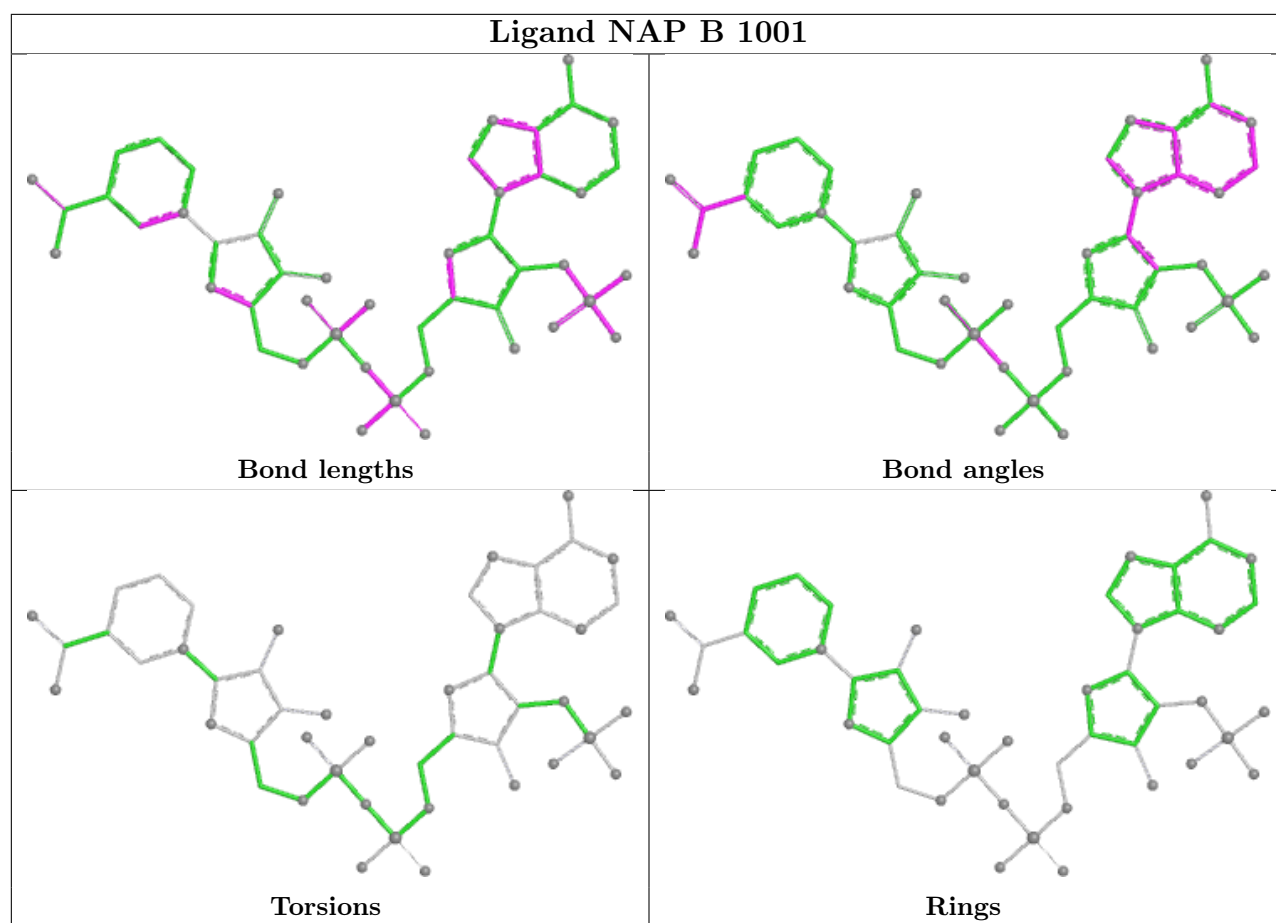
Mol	Chain	Res	Type	Atoms
3	A	1003	NES	C2-C3-N4-C7
3	A	1003	NES	C4-C3-N4-C7
3	A	1003	NES	C6-C3-N4-C7
3	A	1003	NES	O1-C2-C3-N4
3	A	1003	NES	O1-C2-C3-C4
3	A	1003	NES	O1-C2-C3-C6
3	A	1003	NES	C6-C3-C4-O5
3	B	1003	NES	N4-C3-C4-O5
3	B	1003	NES	C2-C3-C4-O5
3	B	1003	NES	C6-C3-C4-O5
3	A	1003	NES	C2-C3-C4-O5
3	A	1003	NES	C8-C7-N4-C3
3	B	1003	NES	C2-C3-N4-C7
3	B	1003	NES	C6-C3-N4-C7
3	B	1003	NES	C8-C7-N4-C3
3	A	1003	NES	N4-C3-C4-O5
3	A	1002	NES	C6-C3-C4-O5
3	A	1003	NES	C7-C8-S-O1S
3	A	1002	NES	N4-C3-C4-O5
3	A	1002	NES	N4-C7-C8-S

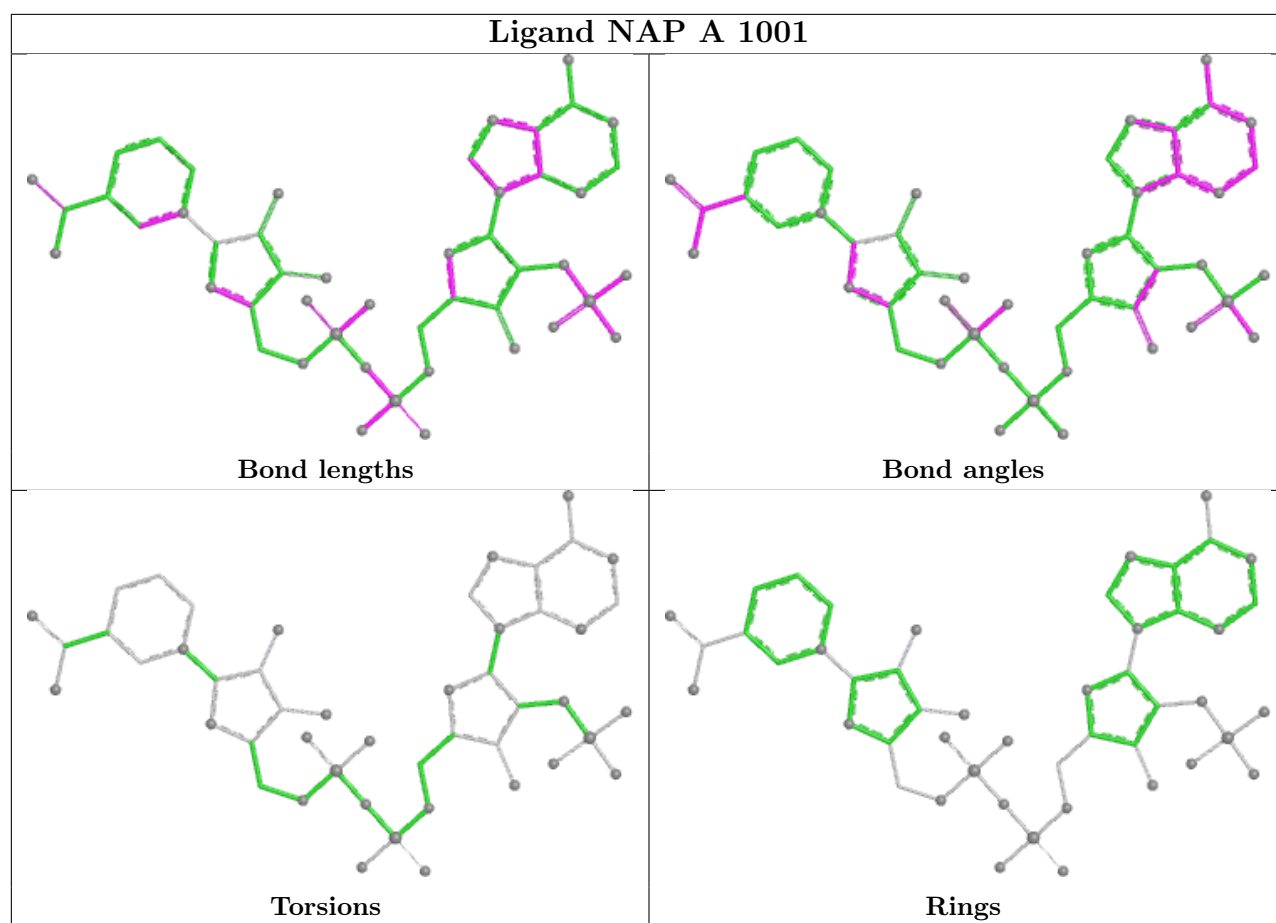
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	NES	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	327/334 (97%)	-1.27	0 100 100	21, 32, 53, 65	0
1	B	327/334 (97%)	-1.27	0 100 100	22, 32, 53, 65	0
All	All	654/668 (97%)	-1.27	0 100 100	21, 32, 53, 65	0

There are no RSRZ outliers to report.

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](#)

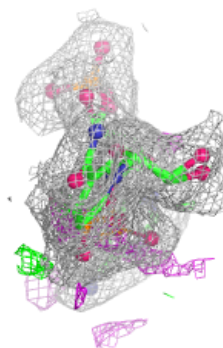
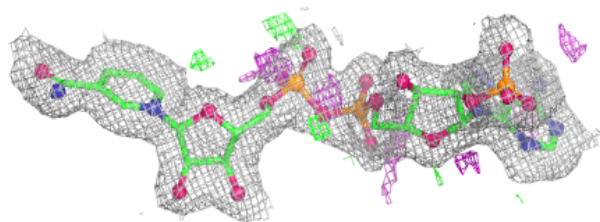
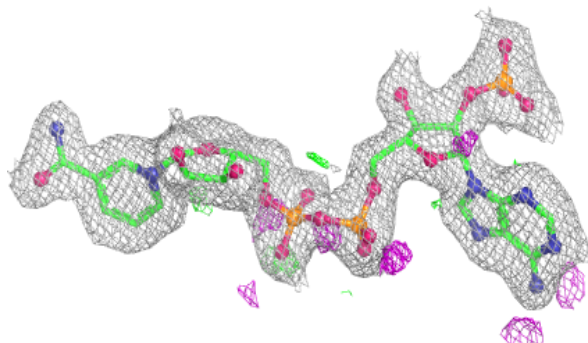
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

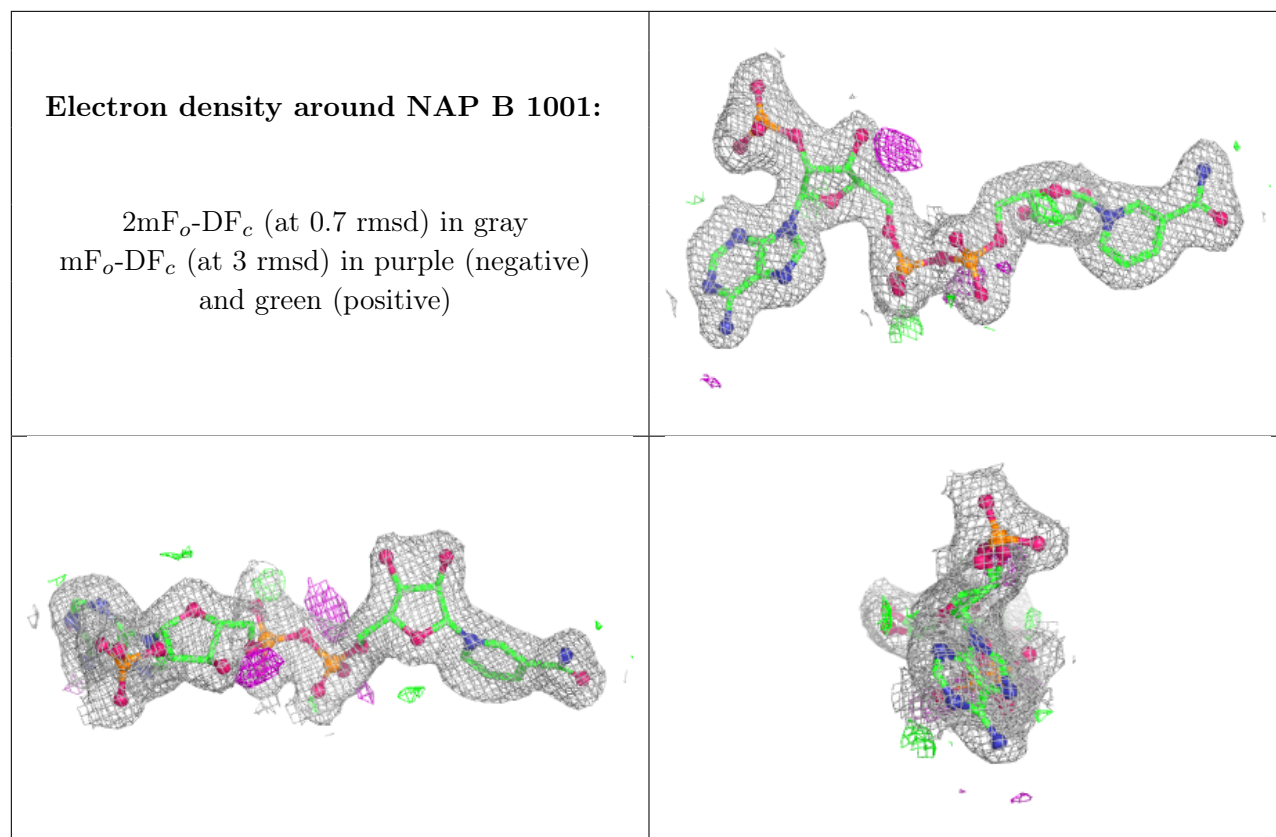
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NES	B	1003	14/14	0.97	0.07	45,66,76,76	0
3	NES	A	1003	14/14	0.98	0.06	45,66,76,77	0
3	NES	A	1002	14/14	0.99	0.05	35,40,45,46	0
2	NAP	A	1001	48/48	0.99	0.03	23,29,35,37	0
3	NES	B	1002	14/14	0.99	0.04	34,40,44,45	0
2	NAP	B	1001	48/48	0.99	0.03	23,30,36,39	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)





6.5 Other polymers [i](#)

There are no such residues in this entry.