



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2025 – 07:07 pm BST

PDB ID : 9GSU / pdb\_00009gsu  
Title : Structure of PP1-Neurabin bound to 4E-BP1.  
Authors : Mouilleron, S.; Treisman, R.; Fedoryshchak, R.; Elbouri, K.  
Deposited on : 2024-09-16  
Resolution : 2.36 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

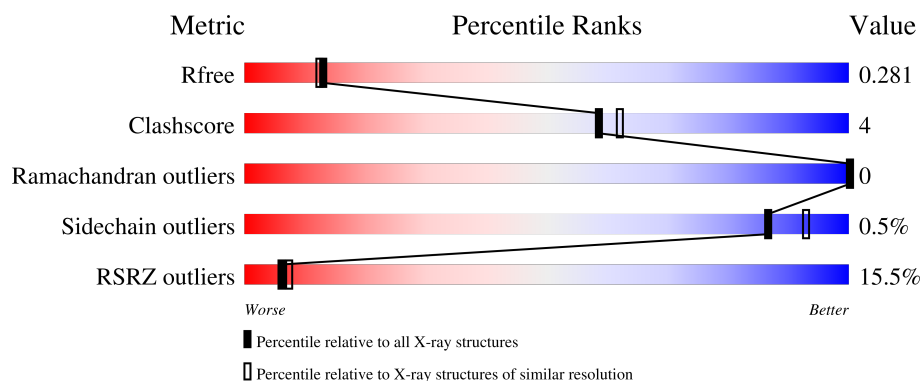
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
$R_{free}$	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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  $\geq 3$ , 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	340	<div> <div>14%</div> <div>77%</div> <div>10%</div> <div>12%</div> </div>
1	D	340	<div> <div>3%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
2	C	176	<div> <div>26%</div> <div>63%</div> <div>13%</div> <div>24%</div> </div>
2	E	176	<div> <div>11%</div> <div>34%</div> <div>•</div> <div>64%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12110 atoms, of which 5930 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 Serine/threonine-protein phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	H	N	O	S	0	0	0
			4577	1505	2236	386	431	19			
1	D	293	Total	C	H	N	O	S	0	1	0
			4621	1504	2280	389	430	18			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP A0A8C3UBZ3
A	3	HIS	-	expression tag	UNP A0A8C3UBZ3
A	4	MET	-	expression tag	UNP A0A8C3UBZ3
A	5	GLY	-	expression tag	UNP A0A8C3UBZ3
A	6	SER	-	expression tag	UNP A0A8C3UBZ3
A	14	GLY	SER	conflict	UNP A0A8C3UBZ3
A	1082	SER	-	expression tag	UNP A0A8C3UBZ3
A	1083	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1084	SER	-	expression tag	UNP A0A8C3UBZ3
A	1085	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1086	SER	-	expression tag	UNP A0A8C3UBZ3
A	1087	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1088	SER	-	expression tag	UNP A0A8C3UBZ3
A	1089	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1090	SER	-	expression tag	UNP A0A8C3UBZ3
A	1091	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1092	SER	-	expression tag	UNP A0A8C3UBZ3
A	1093	PRO	-	expression tag	UNP A0A8C3UBZ3
A	1094	VAL	-	expression tag	UNP A0A8C3UBZ3
A	1095	THR	-	expression tag	UNP A0A8C3UBZ3
A	1096	LYS	-	expression tag	UNP A0A8C3UBZ3
A	1097	THR	-	expression tag	UNP A0A8C3UBZ3
A	1098	PRO	-	expression tag	UNP A0A8C3UBZ3
A	1099	PRO	-	expression tag	UNP A0A8C3UBZ3
A	1100	ARG	-	expression tag	UNP A0A8C3UBZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1101	ASP	-	expression tag	UNP A0A8C3UBZ3
A	1102	LEU	-	expression tag	UNP A0A8C3UBZ3
A	1103	PRO	-	expression tag	UNP A0A8C3UBZ3
A	1104	THR	-	expression tag	UNP A0A8C3UBZ3
A	1105	ILE	-	expression tag	UNP A0A8C3UBZ3
A	1106	PRO	-	expression tag	UNP A0A8C3UBZ3
A	1107	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1108	VAL	-	expression tag	UNP A0A8C3UBZ3
A	1109	THR	-	expression tag	UNP A0A8C3UBZ3
A	1110	SER	-	expression tag	UNP A0A8C3UBZ3
A	1111	GLY	-	expression tag	UNP A0A8C3UBZ3
A	1112	SER	-	expression tag	UNP A0A8C3UBZ3
A	1113	GLN	-	expression tag	UNP A0A8C3UBZ3
A	1114	PHE	-	expression tag	UNP A0A8C3UBZ3
A	1115	GLU	-	expression tag	UNP A0A8C3UBZ3
A	1116	MET	-	expression tag	UNP A0A8C3UBZ3
A	1117	ASP	-	expression tag	UNP A0A8C3UBZ3
A	1118	ILE	-	expression tag	UNP A0A8C3UBZ3
D	2	GLY	-	expression tag	UNP A0A8C3UBZ3
D	3	HIS	-	expression tag	UNP A0A8C3UBZ3
D	4	MET	-	expression tag	UNP A0A8C3UBZ3
D	5	GLY	-	expression tag	UNP A0A8C3UBZ3
D	6	SER	-	expression tag	UNP A0A8C3UBZ3
D	14	GLY	SER	conflict	UNP A0A8C3UBZ3
D	305	SER	-	expression tag	UNP A0A8C3UBZ3
D	306	GLY	-	expression tag	UNP A0A8C3UBZ3
D	307	SER	-	expression tag	UNP A0A8C3UBZ3
D	308	GLY	-	expression tag	UNP A0A8C3UBZ3
D	309	SER	-	expression tag	UNP A0A8C3UBZ3
D	310	GLY	-	expression tag	UNP A0A8C3UBZ3
D	311	SER	-	expression tag	UNP A0A8C3UBZ3
D	312	GLY	-	expression tag	UNP A0A8C3UBZ3
D	313	SER	-	expression tag	UNP A0A8C3UBZ3
D	314	GLY	-	expression tag	UNP A0A8C3UBZ3
D	315	SER	-	expression tag	UNP A0A8C3UBZ3
D	316	PRO	-	expression tag	UNP A0A8C3UBZ3
D	317	VAL	-	expression tag	UNP A0A8C3UBZ3
D	318	THR	-	expression tag	UNP A0A8C3UBZ3
D	319	LYS	-	expression tag	UNP A0A8C3UBZ3
D	320	THR	-	expression tag	UNP A0A8C3UBZ3
D	321	PRO	-	expression tag	UNP A0A8C3UBZ3
D	322	PRO	-	expression tag	UNP A0A8C3UBZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	323	ARG	-	expression tag	UNP A0A8C3UBZ3
D	324	ASP	-	expression tag	UNP A0A8C3UBZ3
D	325	LEU	-	expression tag	UNP A0A8C3UBZ3
D	326	PRO	-	expression tag	UNP A0A8C3UBZ3
D	327	THR	-	expression tag	UNP A0A8C3UBZ3
D	328	ILE	-	expression tag	UNP A0A8C3UBZ3
D	329	PRO	-	expression tag	UNP A0A8C3UBZ3
D	330	GLY	-	expression tag	UNP A0A8C3UBZ3
D	331	VAL	-	expression tag	UNP A0A8C3UBZ3
D	332	THR	-	expression tag	UNP A0A8C3UBZ3
D	333	SER	-	expression tag	UNP A0A8C3UBZ3
D	334	GLY	-	expression tag	UNP A0A8C3UBZ3
D	335	SER	-	expression tag	UNP A0A8C3UBZ3
D	336	GLN	-	expression tag	UNP A0A8C3UBZ3
D	337	PHE	-	expression tag	UNP A0A8C3UBZ3
D	338	GLU	-	expression tag	UNP A0A8C3UBZ3
D	339	MET	-	expression tag	UNP A0A8C3UBZ3
D	340	ASP	-	expression tag	UNP A0A8C3UBZ3
D	341	ILE	-	expression tag	UNP A0A8C3UBZ3

- Molecule 2 is a protein called Neurabin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	133	Total	C	H	N	O	S	0	0	0
			1968	628	978	173	188	1			
2	E	63	Total	C	H	N	O	S	0	0	0
			920	307	436	77	99	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	418	GLY	-	expression tag	UNP Q9ULJ8
C	419	PRO	-	expression tag	UNP Q9ULJ8
C	420	LEU	-	expression tag	UNP Q9ULJ8
C	421	GLY	-	expression tag	UNP Q9ULJ8
C	422	SER	-	expression tag	UNP Q9ULJ8
E	418	GLY	-	expression tag	UNP Q9ULJ8
E	419	PRO	-	expression tag	UNP Q9ULJ8
E	420	LEU	-	expression tag	UNP Q9ULJ8
E	421	GLY	-	expression tag	UNP Q9ULJ8
E	422	SER	-	expression tag	UNP Q9ULJ8

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mn 2	0	0
3	D	2	Total 2	Mn 2	0	0

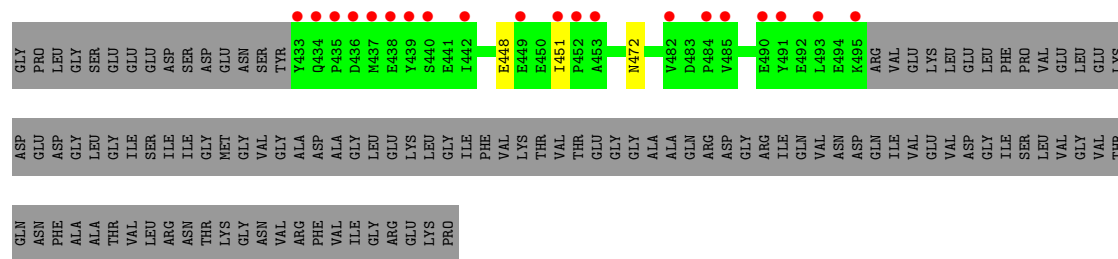
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	D	14	Total 14	O 14	0	0



- Molecule 2: Neurabin-1

Chain E:  11% 34% 64%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.95Å 130.65Å 156.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.48 – 2.36 52.48 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.9 (52.48-2.36) 99.0 (52.48-2.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5058	Depositor
R, $R_{free}$	0.242 , 0.281 0.240 , 0.281	Depositor DCC
$R_{free}$ test set	42437 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8561e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN

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	0.17	0/2395	0.35	0/3243
1	D	0.18	0/2398	0.35	0/3245
2	C	0.15	0/1001	0.30	0/1350
2	E	0.18	0/495	0.29	0/675
All	All	0.17	0/6289	0.34	0/8513

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	2341	2236	2232	25	0
1	D	2341	2280	2280	12	0
2	C	990	978	976	16	0
2	E	484	436	435	2	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	0	0	0
4	D	14	0	0	2	0
All	All	6180	5930	5923	52	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 4.

All (52) 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:D:271:ASN:ND2	2:E:472:ASN:OD1	1.93	1.01
1:D:230:GLU:OE1	4:D:501:HOH:O	1.84	0.95
2:C:464:ILE:HD12	2:C:464:ILE:O	1.86	0.74
2:C:546:GLN:OE1	2:C:546:GLN:C	2.39	0.66
1:D:215:GLY:N	4:D:501:HOH:O	2.16	0.57
2:C:563:ILE:HG21	2:C:576:VAL:HG21	1.91	0.53
1:D:197:ASP:OD1	1:D:197:ASP:N	2.37	0.51
1:A:74:ARG:HD3	1:A:77:GLU:OE1	2.10	0.51
1:A:1116:MET:HE2	1:A:1118:ILE:HG22	1.94	0.50
1:D:96:ARG:NE	1:D:272:TYR:OH	2.45	0.49
2:C:581:LYS:CD	2:C:581:LYS:C	2.86	0.49
2:C:510:ASP:OD2	2:C:510:ASP:C	2.56	0.48
1:D:174:GLY:O	1:D:246:ARG:HD2	2.13	0.48
1:A:239:HIS:HB2	1:A:241:LEU:CD2	2.43	0.48
2:C:531:LYS:C	2:C:532:LEU:HD12	2.39	0.48
1:A:176:LEU:HD21	1:A:244:ILE:HD13	1.96	0.48
2:C:564:SER:OG	2:C:566:VAL:HG22	2.14	0.47
1:A:289:LEU:HD23	2:C:457:ILE:HG22	1.97	0.47
1:A:246:ARG:NH1	1:A:249:GLN:OE1	2.40	0.47
2:C:510:ASP:OD2	2:C:512:ASP:N	2.48	0.47
1:A:247:ALA:O	1:A:248:HIS:HB3	2.15	0.46
2:C:469:THR:HG22	2:C:470:TYR:N	2.29	0.46
1:D:230:GLU:CD	1:D:230:GLU:H	2.23	0.46
2:C:483:ASP:OD1	2:C:485:VAL:HG12	2.15	0.46
1:D:94:VAL:O	1:D:95:ASP:HB2	2.16	0.45
1:D:236:LEU:HD21	1:D:244:ILE:HG13	1.98	0.45
2:C:546:GLN:OE1	2:C:547:ARG:N	2.49	0.44
1:A:236:LEU:HD21	1:A:244:ILE:HG13	2.00	0.44
1:A:60:LYS:HA	1:A:283:MET:O	2.17	0.44
1:A:283:MET:CE	1:A:293:PHE:CE2	3.00	0.44
1:A:75:LEU:C	1:A:75:LEU:HD23	2.43	0.44
1:A:94:VAL:O	1:A:95:ASP:HB2	2.18	0.44
2:C:581:LYS:C	2:C:581:LYS:HD2	2.43	0.44
1:A:89:PHE:HB3	1:A:93:TYR:HE1	1.83	0.43
1:D:247:ALA:O	1:D:248:HIS:HB3	2.18	0.43
1:D:164:ILE:HA	1:D:169:ILE:O	2.18	0.43
1:A:286:ASP:OD1	1:A:288:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG23	1:A:88:LEU:CD2	2.48	0.43
1:A:61:ILE:HG23	1:A:88:LEU:HD23	2.01	0.43
1:A:74:ARG:HH11	1:A:74:ARG:HG3	1.83	0.42
1:A:1114:PHE:O	2:C:519:ILE:HA	2.20	0.42
1:D:131:ASN:HB2	1:D:136:PHE:HB3	2.01	0.42
1:A:131:ASN:HB2	1:A:136:PHE:HB3	2.02	0.42
2:C:530:GLU:O	2:C:532:LEU:HD13	2.19	0.42
1:A:164:ILE:CG2	1:A:167:GLU:HA	2.50	0.42
1:A:283:MET:HE2	1:A:293:PHE:CE2	2.55	0.42
1:A:255:TYR:CD2	1:A:293:PHE:CE2	3.08	0.42
1:A:232:VAL:HG13	1:A:244:ILE:HD12	2.00	0.41
1:A:236:LEU:CD1	1:A:262:GLN:HB3	2.51	0.40
1:A:74:ARG:HD3	1:A:74:ARG:HA	1.88	0.40
2:E:448:GLU:HG3	2:E:451:ILE:HG12	2.03	0.40
2:C:501:GLU:HB2	2:C:592:LYS:HG3	2.04	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	294/340 (86%)	280 (95%)	14 (5%)	0	100	100
1	D	292/340 (86%)	279 (96%)	13 (4%)	0	100	100
2	C	129/176 (73%)	125 (97%)	4 (3%)	0	100	100
2	E	61/176 (35%)	59 (97%)	2 (3%)	0	100	100
All	All	776/1032 (75%)	743 (96%)	33 (4%)	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	246/295 (83%)	244 (99%)	2 (1%)	79	88
1	D	252/295 (85%)	252 (100%)	0	100	100
2	C	99/148 (67%)	98 (99%)	1 (1%)	73	84
2	E	49/148 (33%)	49 (100%)	0	100	100
All	All	646/886 (73%)	643 (100%)	3 (0%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	246	ARG
2	C	591	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	117	ASN
1	A	262	GLN
2	E	479	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/340 (87%)	1.11	47 (15%) 6 7	40, 62, 87, 96	3 (1%)
1	D	293/340 (86%)	0.49	10 (3%) 48 54	30, 49, 66, 87	5 (1%)
2	C	133/176 (75%)	1.63	45 (33%) 1 1	54, 81, 96, 104	5 (3%)
2	E	63/176 (35%)	1.57	20 (31%) 1 1	52, 76, 97, 101	1 (1%)
All	All	787/1032 (76%)	1.01	122 (15%) 6 7	30, 59, 91, 104	14 (1%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	465	LYS	6.1
2	C	512	ASP	5.9
1	A	288	THR	4.8
2	C	464	ILE	4.7
1	A	7	LEU	4.6
1	A	293	PHE	4.5
2	C	544	ALA	4.5
2	C	514	LEU	4.4
1	A	283	MET	4.3
2	C	463	PRO	4.2
2	E	435	PRO	4.2
1	A	287	GLU	3.9
2	E	438	GLU	3.9
1	A	1118	ILE	3.8
1	A	1114	PHE	3.8
2	E	452	PRO	3.8
1	D	7	LEU	3.7
2	C	539	VAL	3.7
1	A	285	VAL	3.6
2	C	461	SER	3.6
1	A	274	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	493	LEU	3.5
2	E	437	MET	3.5
2	C	454	ASN	3.5
2	C	460	SER	3.4
1	A	295	ILE	3.4
2	C	467	PHE	3.3
2	C	511	GLU	3.3
2	C	472	ASN	3.3
2	E	436	ASP	3.3
2	C	480	ASP	3.3
2	C	469	THR	3.2
1	A	178	PRO	3.2
2	E	491	TYR	3.2
1	A	296	LEU	3.2
1	A	63	GLY	3.2
1	A	1113	GLN	3.0
1	D	73	LEU	3.0
1	D	161	ILE	3.0
1	A	228	GLY	3.0
2	C	466	VAL	3.0
2	E	482	VAL	2.9
1	A	237	HIS	2.9
2	C	560	VAL	2.9
2	C	508	GLU	2.9
2	E	449	GLU	2.9
1	A	1115	GLU	2.8
2	C	481	GLU	2.8
2	E	434	GLN	2.8
1	A	79	GLY	2.8
2	C	462	ALA	2.8
2	C	520	GLY	2.8
1	A	255	TYR	2.7
2	C	521	MET	2.6
2	E	442	ILE	2.6
1	D	299	ALA	2.6
1	A	167	GLU	2.6
1	A	273	CYS	2.6
2	E	433	TYR	2.5
2	C	470	TYR	2.5
1	D	230	GLU	2.5
1	A	266	LEU	2.5
1	A	190	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	260	LYS	2.5
2	E	451	ILE	2.4
2	C	530	GLU	2.4
2	C	459	PHE	2.4
2	C	522	GLY	2.4
1	A	75	LEU	2.4
1	A	165	VAL	2.4
2	C	541	GLU	2.4
1	D	176	LEU	2.4
1	A	253	ASP	2.4
2	C	540	THR	2.3
2	C	583	ASN	2.3
2	E	453	ALA	2.3
1	A	169	ILE	2.3
2	C	474	ASP	2.3
2	C	563	ILE	2.3
1	A	55	LEU	2.3
2	C	485	VAL	2.3
1	A	78	TYR	2.3
2	E	495	LYS	2.3
2	E	490	GLU	2.3
1	A	213	VAL	2.3
1	A	251	VAL	2.3
1	A	146	ILE	2.3
1	A	240	ASP	2.3
2	C	457	ILE	2.3
2	C	498	GLU	2.2
2	E	484	PRO	2.2
1	A	245	CYS	2.2
2	C	567	GLY	2.2
2	C	473	GLU	2.2
2	E	485	VAL	2.2
1	A	84	GLU	2.2
2	C	513	GLY	2.2
2	C	518	ILE	2.2
1	A	23	ARG	2.2
1	A	8	ASN	2.2
1	A	201	LEU	2.2
2	E	439	TYR	2.2
2	C	517	SER	2.1
2	E	440	SER	2.1
1	A	80	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	291	CYS	2.1
1	D	274	GLY	2.1
1	A	298	PRO	2.1
2	C	486	ALA	2.1
1	D	273	CYS	2.1
1	A	59	LEU	2.1
1	D	21	GLY	2.1
2	C	471	SER	2.1
2	C	582	GLY	2.1
2	C	519	ILE	2.1
2	C	479	ASN	2.1
1	D	96	ARG	2.1
1	A	188	ARG	2.0
2	C	566	VAL	2.0
1	A	96	ARG	2.0
1	A	162	ALA	2.0
1	A	281	ALA	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, 95<sup>th</sup> 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.

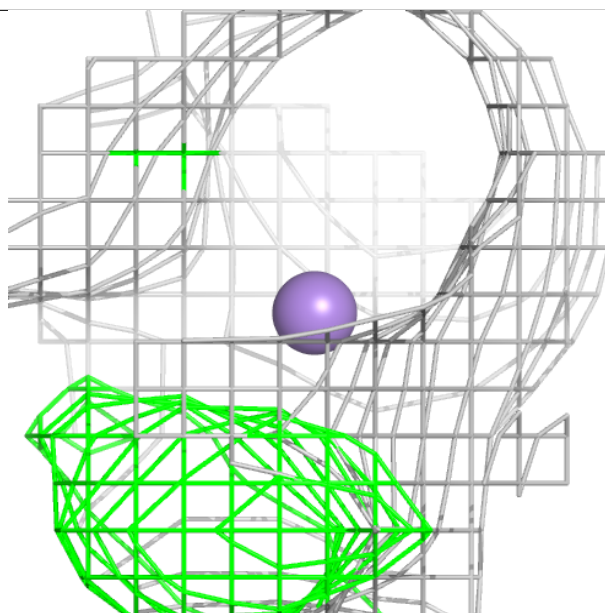
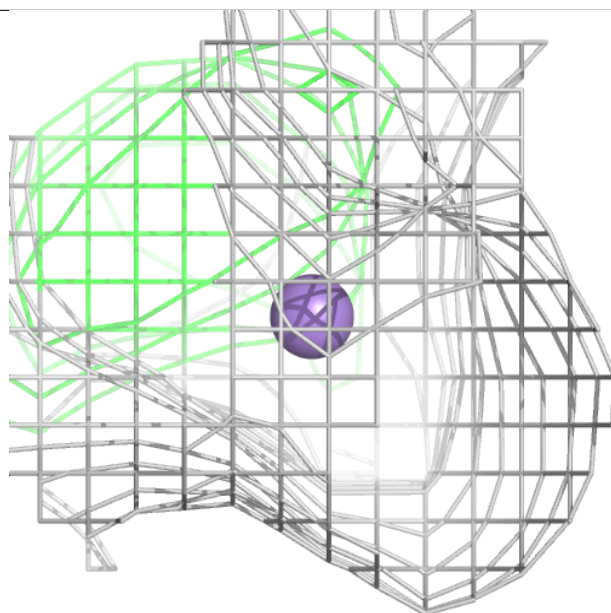
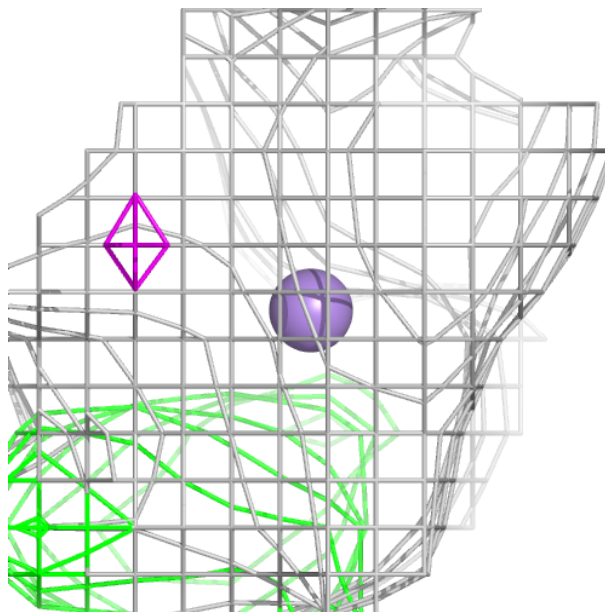
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	D	401	1/1	0.83	0.12	87,87,87,87	0
3	MN	A	1202	1/1	0.90	0.07	90,90,90,90	0
3	MN	A	1201	1/1	0.95	0.07	51,51,51,51	0
3	MN	D	402	1/1	0.98	0.04	43,43,43,43	0

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.

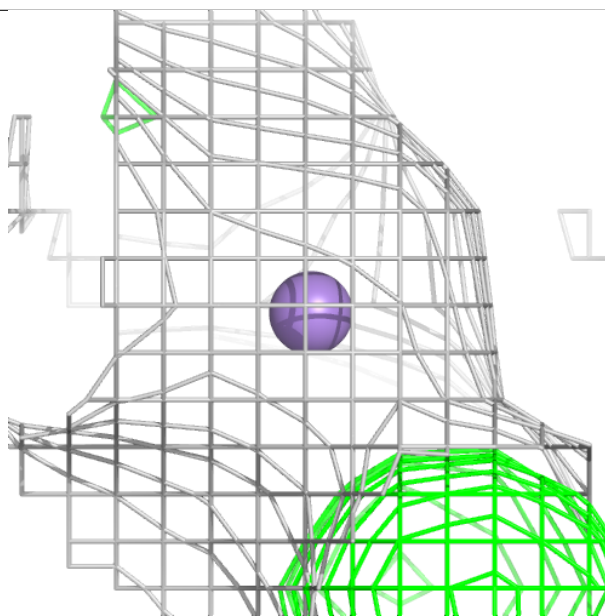
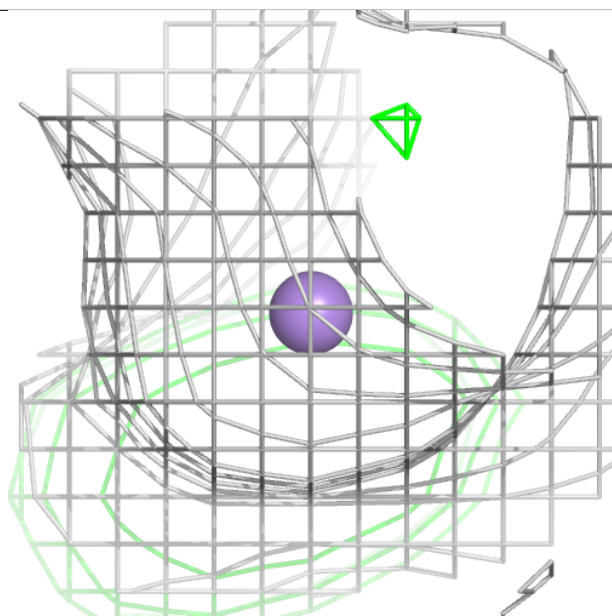
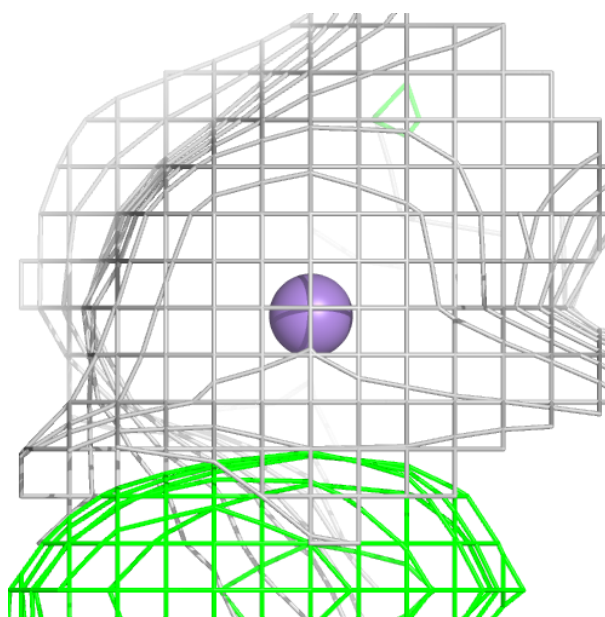
**Electron density around MN D 401:**

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



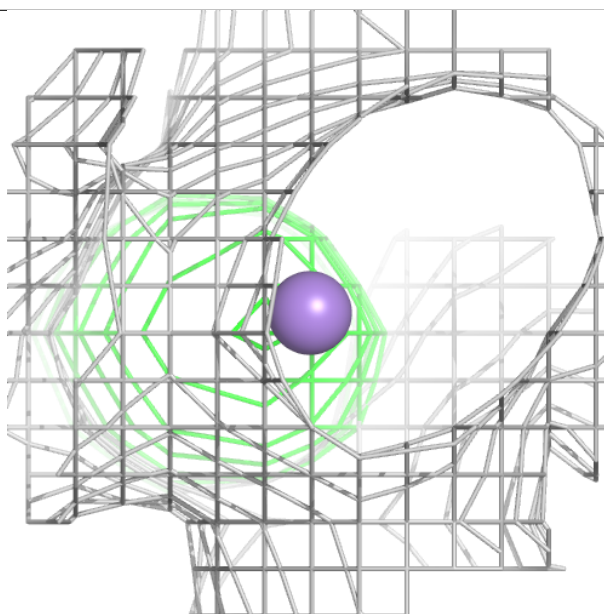
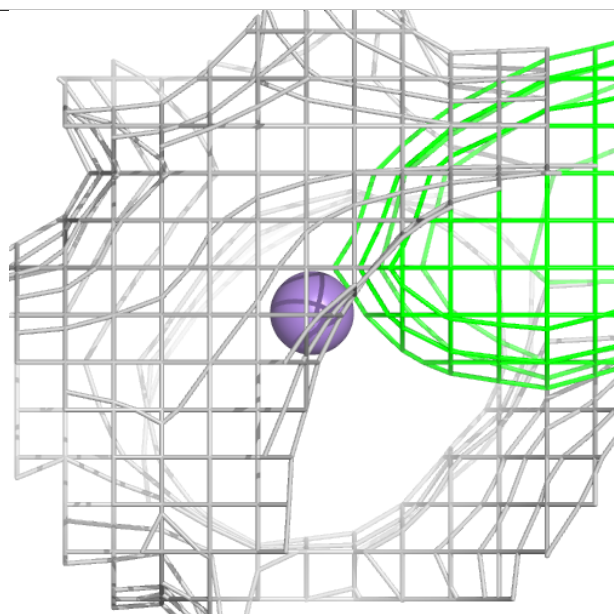
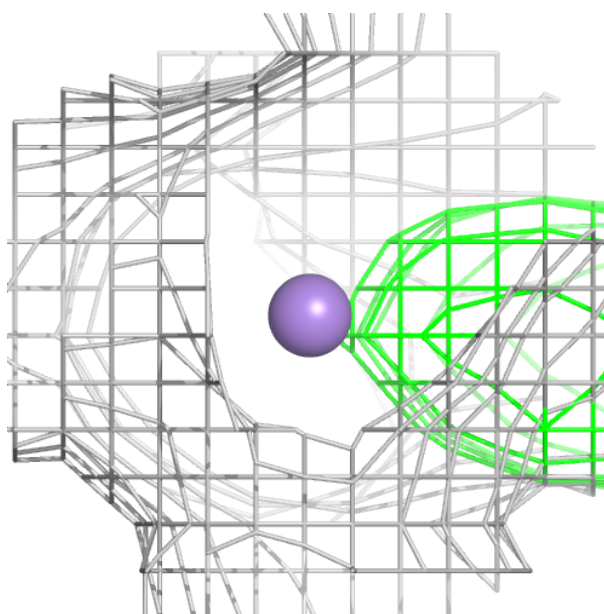
**Electron density around MN A 1202:**

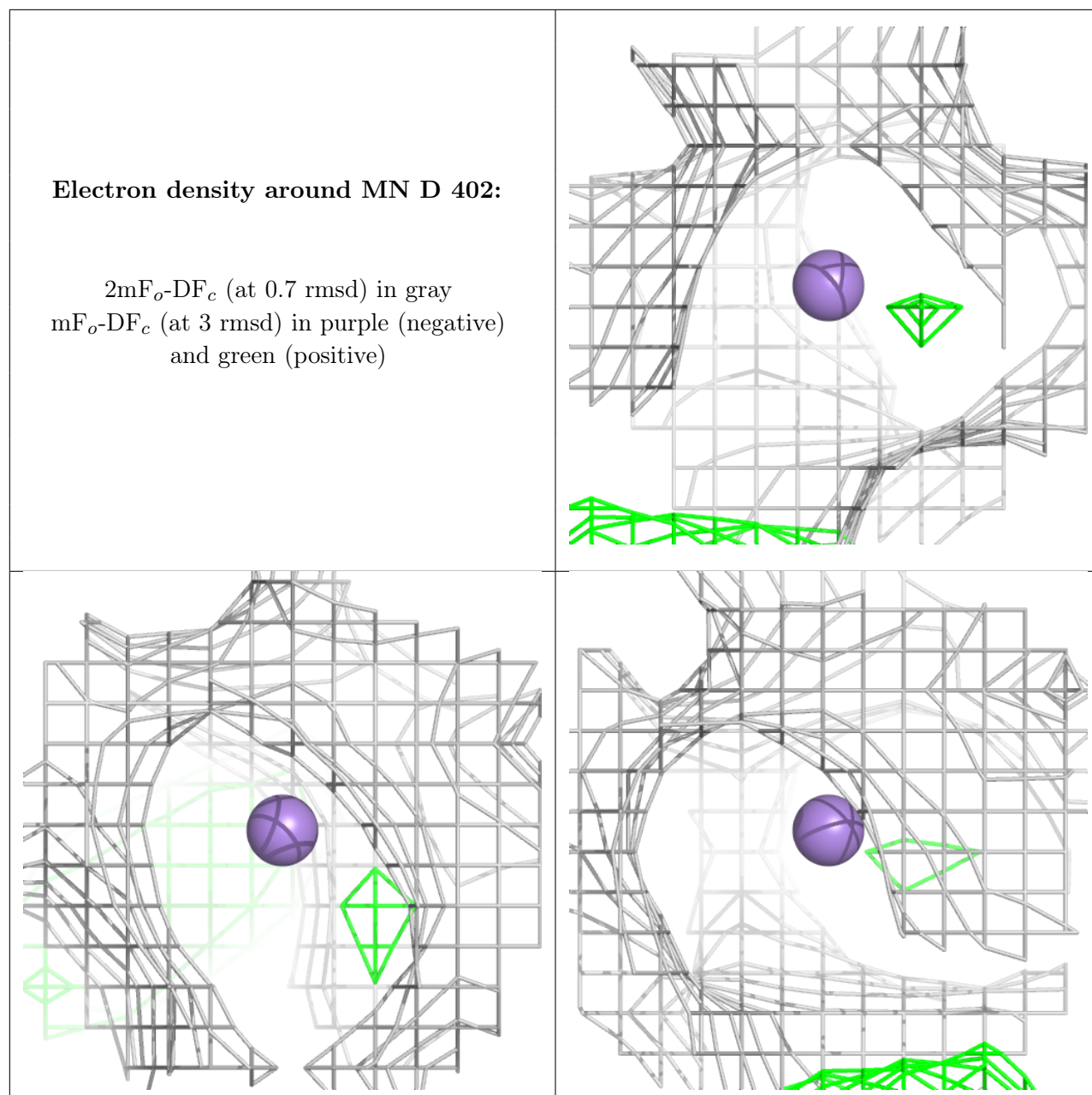
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MN A 1201:**

$2mF_o-DF_c$  (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.