



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 13, 2026 – 02:37 pm BST

PDB ID : 2VUS / pdb_00002vus
Title : Crystal structure of unliganded NmrA-AreA zinc finger complex
Authors : Kotaka, M.; Johnson, C.; Lamb, H.K.; Hawkins, A.R.; Ren, J.; Stammers, D.K.
Deposited on : 2008-05-30
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

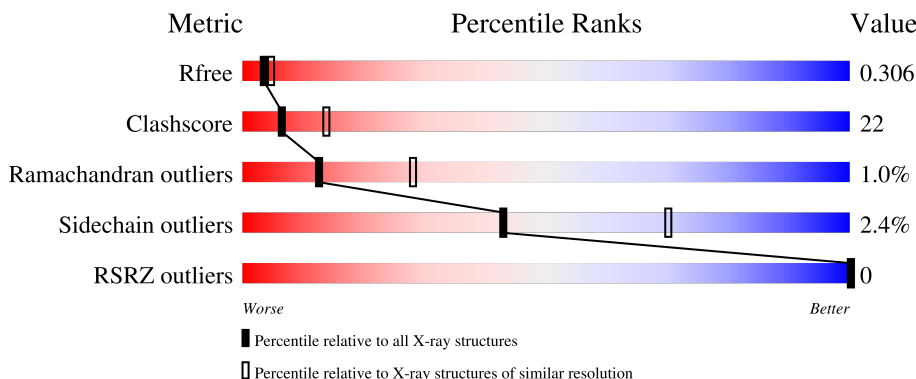
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	352	
1	B	352	
1	C	352	
1	D	352	
1	E	352	

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Mol	Chain	Length	Quality of chain
1	F	352	 57% 31% • 10%
1	G	352	 57% 30% • 10%
1	H	352	 55% 31% • 10%
2	I	43	 60% 33% 5% •
2	J	43	 56% 40% • •
2	K	43	 51% 37% 7% 5%
2	L	43	 53% 42% • •
2	M	43	 63% 35% •
2	N	43	 58% 37% • •
2	O	43	 63% 30% • 5%
2	P	43	 60% 35% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24506 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 NITROGEN METABOLITE REPRESSION REGULATOR NMRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	B	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	C	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	D	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	E	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	F	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	G	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	H	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			

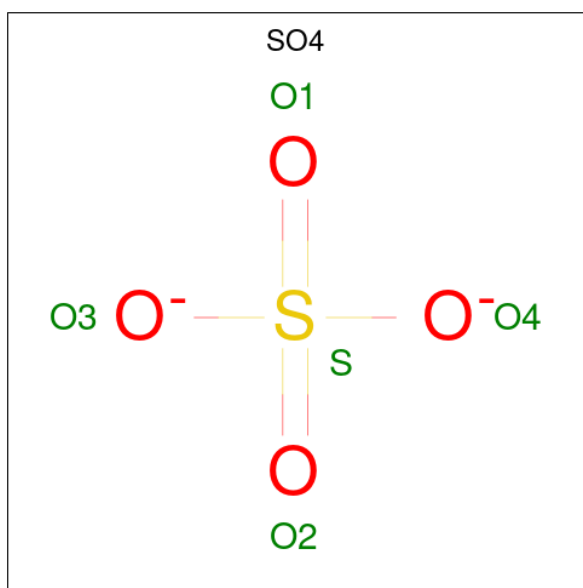
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ARG	LEU	conflict	UNP O59919
B	238	ARG	LEU	conflict	UNP O59919
C	238	ARG	LEU	conflict	UNP O59919
D	238	ARG	LEU	conflict	UNP O59919
E	238	ARG	LEU	conflict	UNP O59919
F	238	ARG	LEU	conflict	UNP O59919
G	238	ARG	LEU	conflict	UNP O59919
H	238	ARG	LEU	conflict	UNP O59919

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN AREA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	J	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	K	41	Total	C	N	O	S	0	0	0
			318	200	59	55	4			
2	L	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	M	43	Total	C	N	O	S	0	0	0
			333	211	61	57	4			
2	N	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	O	41	Total	C	N	O	S	0	0	0
			318	200	59	55	4			
2	P	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	2	Total	Cl	0	0
			2	2		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Zn	0	0
			1	1		
5	J	1	Total	Zn	0	0
			1	1		
5	K	1	Total	Zn	0	0
			1	1		
5	L	1	Total	Zn	0	0
			1	1		
5	M	1	Total	Zn	0	0
			1	1		
5	N	1	Total	Zn	0	0
			1	1		
5	O	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Zn	0	0
			1	1		

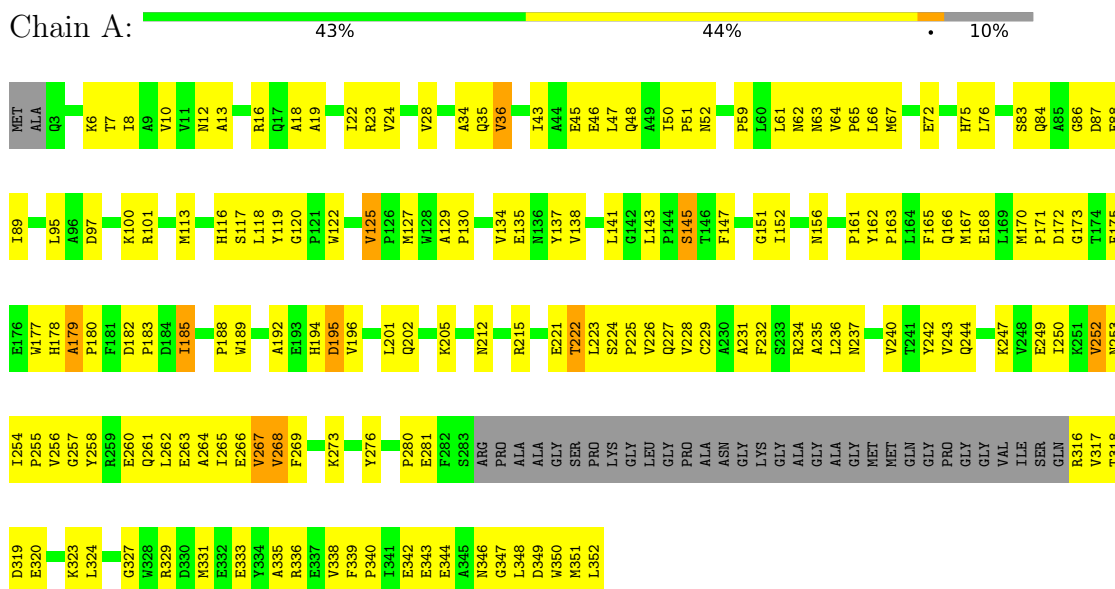
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	181	Total	O	0	0
			181	181		
6	C	192	Total	O	0	0
			192	192		
6	D	184	Total	O	0	0
			184	184		
6	E	207	Total	O	0	0
			207	207		
6	F	170	Total	O	0	0
			170	170		
6	G	212	Total	O	0	0
			212	212		
6	H	177	Total	O	0	0
			177	177		
6	I	26	Total	O	0	0
			26	26		
6	J	17	Total	O	0	0
			17	17		
6	K	20	Total	O	0	0
			20	20		
6	L	16	Total	O	0	0
			16	16		
6	M	17	Total	O	0	0
			17	17		
6	N	17	Total	O	0	0
			17	17		
6	O	17	Total	O	0	0
			17	17		
6	P	11	Total	O	0	0
			11	11		

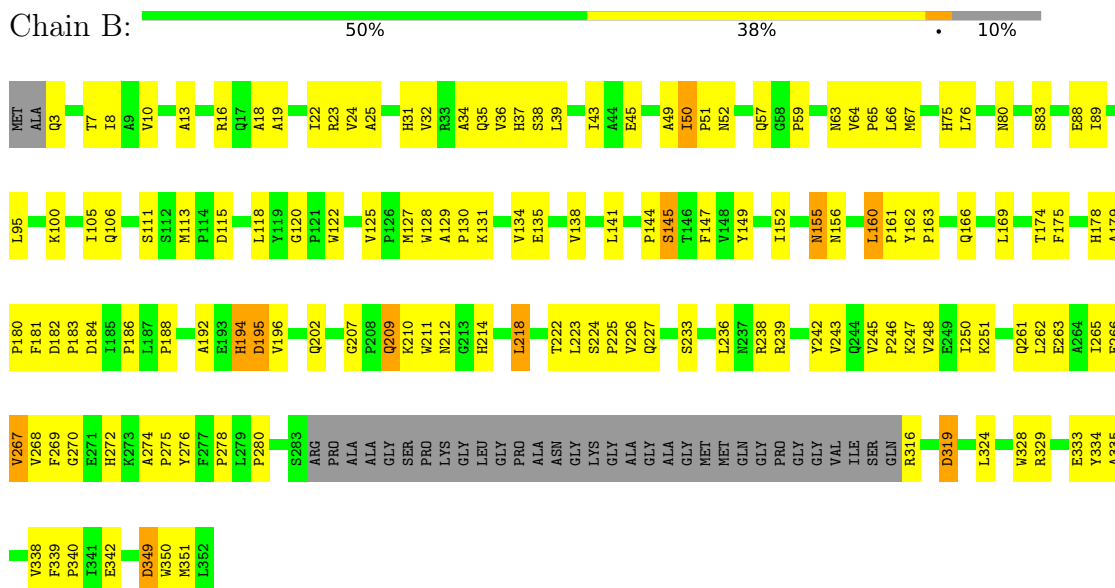
3 Residue-property plots

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.

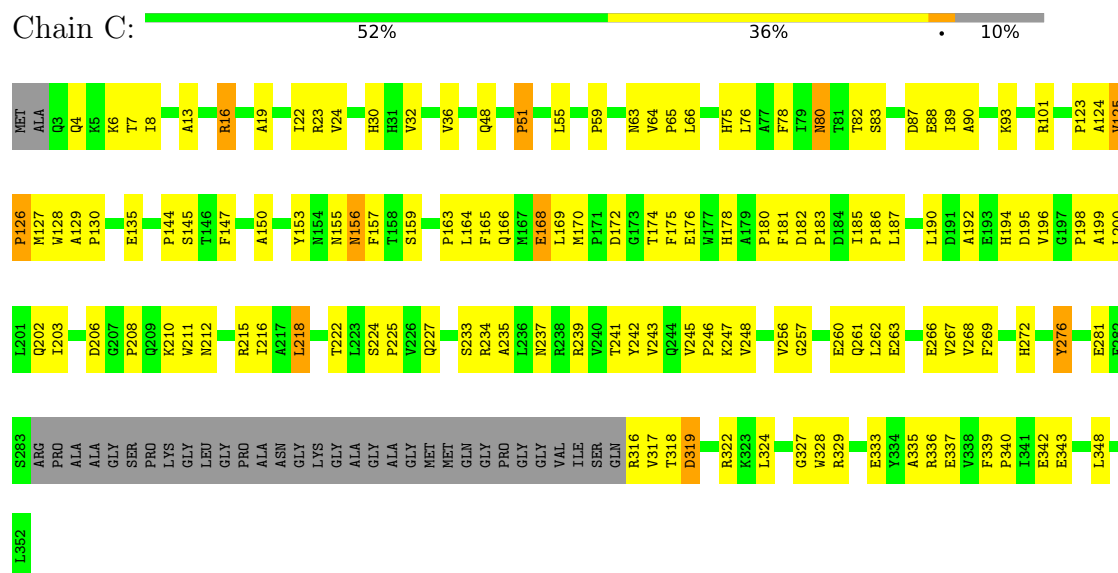
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA



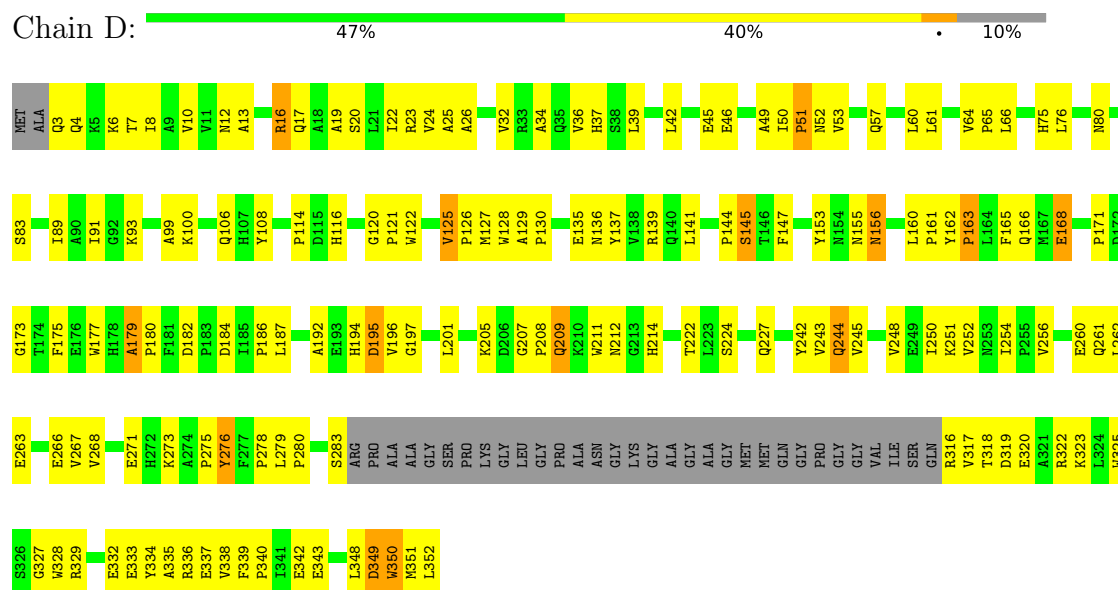
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA



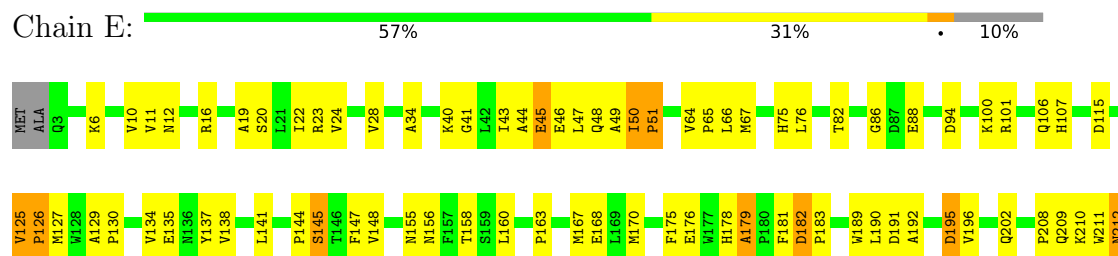
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

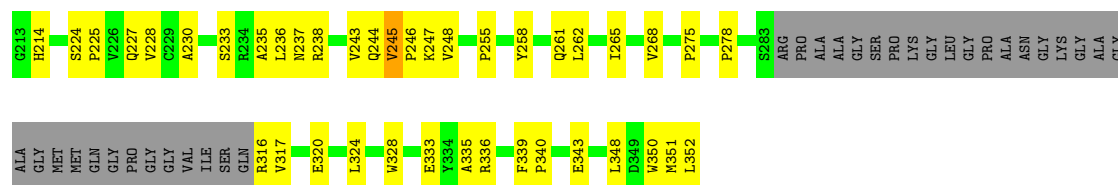


• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA



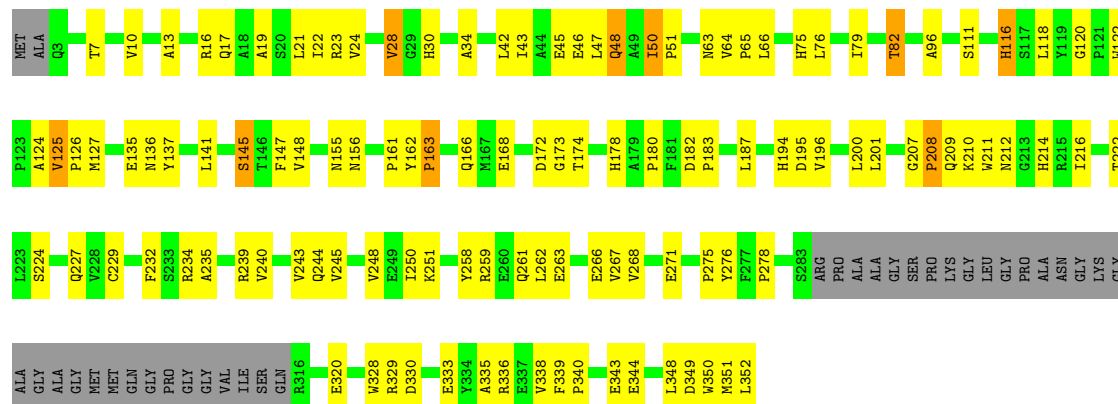
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA





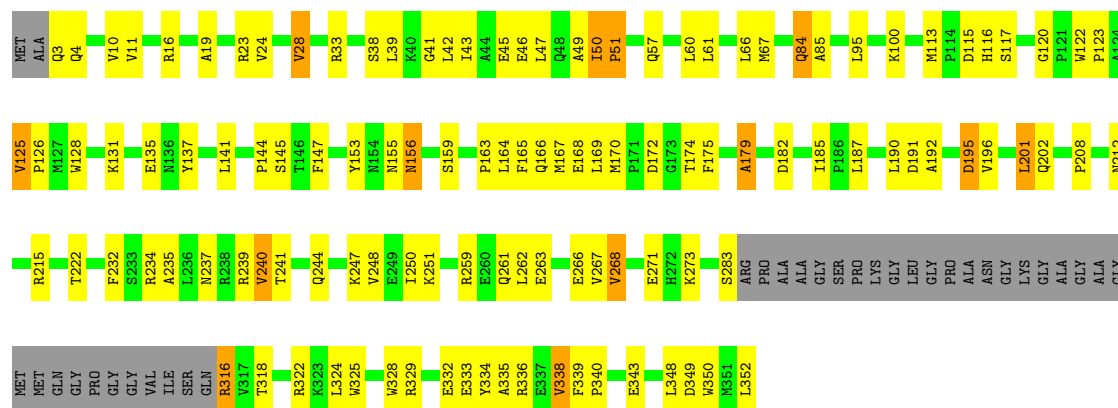
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain F: 57% 31% 10%



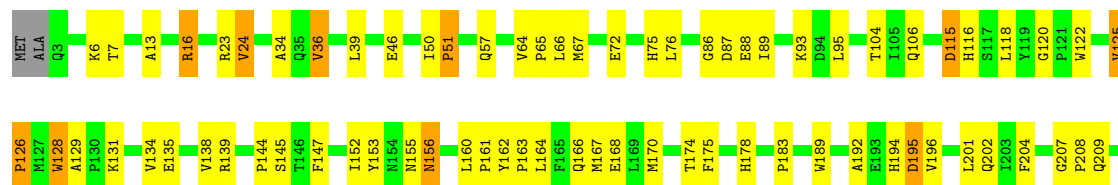
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

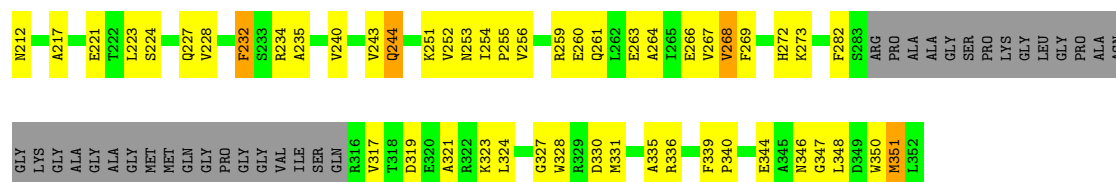
Chain G: 57% 30% 10%



• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

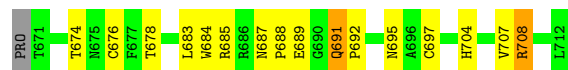
Chain H: 55% 31% 10%





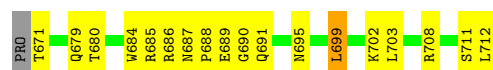
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain I: 60% 33% 5%



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain J: 56% 40% 4%



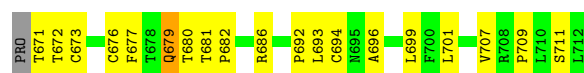
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain K: 51% 37% 7% 5%



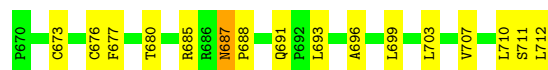
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain L: 53% 42% 5%



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain M: 63% 35% 2%



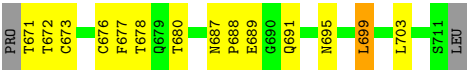
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain N: 58% 37% 5%



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain O: 63% 30% • 5%



● Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain P: 60% 35% • •



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	228.79Å 228.79Å 222.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 2.60 29.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.97-2.60) 98.8 (29.97-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.306 0.243 , 0.306	Depositor DCC
R_{free} test set	6691 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 8.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.387 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24506	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.13% 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: CL, ZN, SO4

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	0.43	0/2606	1.01	20/3557 (0.6%)
1	B	0.45	0/2606	1.04	19/3557 (0.5%)
1	C	0.48	0/2606	0.99	13/3557 (0.4%)
1	D	0.46	0/2606	1.03	16/3557 (0.4%)
1	E	0.47	0/2606	1.06	16/3557 (0.4%)
1	F	0.44	0/2606	0.99	13/3557 (0.4%)
1	G	0.46	0/2606	1.03	17/3557 (0.5%)
1	H	0.46	1/2606 (0.0%)	1.03	18/3557 (0.5%)
2	I	0.47	0/334	1.04	4/456 (0.9%)
2	J	0.43	0/334	0.96	0/456
2	K	0.43	0/326	0.96	0/445
2	L	0.41	0/334	0.84	1/456 (0.2%)
2	M	0.46	0/342	0.89	1/467 (0.2%)
2	N	0.49	0/334	0.97	2/456 (0.4%)
2	O	0.45	0/326	0.85	0/445
2	P	0.45	0/334	0.90	0/456
All	All	0.46	1/23512 (0.0%)	1.01	140/32093 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	128	TRP	CA-C	5.13	1.56	1.52

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	VAL	CA-C-N	8.91	130.98	119.84
1	E	125	VAL	C-N-CA	8.91	130.98	119.84
1	A	185	ILE	N-CA-C	8.87	115.64	107.56
1	F	125	VAL	CA-C-N	8.03	129.88	119.84
1	F	125	VAL	C-N-CA	8.03	129.88	119.84

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	2530	0	2476	139	0
1	B	2530	0	2476	112	0
1	C	2530	0	2476	107	0
1	D	2530	0	2476	130	0
1	E	2530	0	2476	100	0
1	F	2530	0	2476	105	0
1	G	2530	0	2476	95	0
1	H	2530	0	2476	105	0
2	I	326	0	326	11	0
2	J	326	0	326	19	0
2	K	318	0	315	27	0
2	L	326	0	326	16	0
2	M	333	0	334	11	0
2	N	326	0	326	15	0
2	O	318	0	315	15	0
2	P	326	0	326	12	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
6	A	148	0	0	11	0
6	B	181	0	0	16	0
6	C	192	0	0	13	0
6	D	184	0	0	18	0
6	E	207	0	0	11	0
6	F	170	0	0	9	0
6	G	212	0	0	19	0
6	H	177	0	0	8	0
6	I	26	0	0	0	0
6	J	17	0	0	3	0
6	K	20	0	0	0	0
6	L	16	0	0	3	0
6	M	17	0	0	0	0
6	N	17	0	0	3	0
6	O	17	0	0	0	0
6	P	11	0	0	0	0
All	All	24506	0	22402	991	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 22.

The worst 5 of 991 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)
2:J:687:ASN:HD21	2:J:691:GLN:HB2	1.14	1.06
1:G:352:LEU:OXT	6:G:2212:HOH:O	1.72	1.06
2:N:687:ASN:HD22	2:N:691:GLN:HB2	1.17	1.05
1:A:261:GLN:HE21	1:A:265:ILE:HD11	1.21	1.04
2:O:687:ASN:HD21	2:O:691:GLN:HB2	1.19	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/352 (89%)	291 (93%)	20 (6%)	3 (1%)	12	28
1	B	314/352 (89%)	287 (91%)	24 (8%)	3 (1%)	12	28
1	C	314/352 (89%)	290 (92%)	22 (7%)	2 (1%)	21	42
1	D	314/352 (89%)	292 (93%)	19 (6%)	3 (1%)	12	28
1	E	314/352 (89%)	285 (91%)	27 (9%)	2 (1%)	21	42
1	F	314/352 (89%)	280 (89%)	33 (10%)	1 (0%)	36	58
1	G	314/352 (89%)	294 (94%)	18 (6%)	2 (1%)	21	42
1	H	314/352 (89%)	288 (92%)	21 (7%)	5 (2%)	7	16
2	I	40/43 (93%)	37 (92%)	2 (5%)	1 (2%)	4	8
2	J	40/43 (93%)	36 (90%)	3 (8%)	1 (2%)	4	8
2	K	39/43 (91%)	35 (90%)	3 (8%)	1 (3%)	4	7
2	L	40/43 (93%)	31 (78%)	8 (20%)	1 (2%)	4	8
2	M	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
2	N	40/43 (93%)	37 (92%)	3 (8%)	0	100	100
2	O	39/43 (91%)	37 (95%)	1 (3%)	1 (3%)	4	7
2	P	40/43 (93%)	38 (95%)	1 (2%)	1 (2%)	4	8
All	All	2831/3160 (90%)	2596 (92%)	208 (7%)	27 (1%)	12	28

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	TRP
1	G	116	HIS
1	A	253	ASN
1	B	319	ASP
1	F	350	TRP

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	266/284 (94%)	256 (96%)	10 (4%)	29	56
1	B	266/284 (94%)	260 (98%)	6 (2%)	44	71
1	C	266/284 (94%)	262 (98%)	4 (2%)	57	80
1	D	266/284 (94%)	260 (98%)	6 (2%)	44	71
1	E	266/284 (94%)	260 (98%)	6 (2%)	44	71
1	F	266/284 (94%)	263 (99%)	3 (1%)	65	84
1	G	266/284 (94%)	260 (98%)	6 (2%)	44	71
1	H	266/284 (94%)	260 (98%)	6 (2%)	44	71
2	I	38/39 (97%)	37 (97%)	1 (3%)	40	68
2	J	38/39 (97%)	37 (97%)	1 (3%)	40	68
2	K	37/39 (95%)	35 (95%)	2 (5%)	20	42
2	L	38/39 (97%)	37 (97%)	1 (3%)	40	68
2	M	39/39 (100%)	37 (95%)	2 (5%)	21	45
2	N	38/39 (97%)	37 (97%)	1 (3%)	40	68
2	O	37/39 (95%)	34 (92%)	3 (8%)	11	24
2	P	38/39 (97%)	37 (97%)	1 (3%)	40	68
All	All	2431/2584 (94%)	2372 (98%)	59 (2%)	43	70

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	51	PRO
2	O	671	THR
1	G	28	VAL
2	N	707	VAL
2	K	683	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	106	GLN
1	G	107	HIS
2	N	687	ASN
1	F	166	GLN
1	F	253	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 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	SO4	G	1353	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	D	1353	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	E	1353	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	H	1353	-	4,4,4	0.26	0	6,6,6	0.21	0
3	SO4	C	1353	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	A	1353	-	4,4,4	0.39	0	6,6,6	0.18	0
3	SO4	F	1353	-	4,4,4	0.26	0	6,6,6	0.22	0
3	SO4	B	1353	-	4,4,4	0.30	0	6,6,6	0.17	0

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 [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	318/352 (90%)	-1.49	0 100 100	8, 28, 61, 91	0
1	B	318/352 (90%)	-1.43	0 100 100	9, 26, 53, 73	0
1	C	318/352 (90%)	-1.56	0 100 100	10, 22, 45, 69	0
1	D	318/352 (90%)	-1.50	0 100 100	10, 26, 57, 72	0
1	E	318/352 (90%)	-1.55	0 100 100	8, 24, 52, 75	0
1	F	318/352 (90%)	-1.47	0 100 100	9, 25, 55, 70	0
1	G	318/352 (90%)	-1.57	0 100 100	5, 23, 50, 75	0
1	H	318/352 (90%)	-1.54	0 100 100	7, 24, 59, 82	0
2	I	42/43 (97%)	-1.22	0 100 100	8, 33, 92, 111	0
2	J	42/43 (97%)	-1.27	0 100 100	14, 37, 89, 101	0
2	K	41/43 (95%)	-1.31	0 100 100	12, 37, 100, 104	0
2	L	42/43 (97%)	-1.21	0 100 100	16, 41, 96, 119	0
2	M	43/43 (100%)	-1.24	0 100 100	13, 35, 101, 116	0
2	N	42/43 (97%)	-1.34	0 100 100	9, 31, 90, 110	0
2	O	41/43 (95%)	-1.31	0 100 100	20, 34, 89, 106	0
2	P	42/43 (97%)	-1.28	0 100 100	14, 39, 99, 107	0
All	All	2879/3160 (91%)	-1.49	0 100 100	5, 26, 59, 119	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1353	5/5	0.98	0.04	30,31,52,71	0
4	CL	A	1354	1/1	0.98	0.11	58,58,58,58	0
3	SO4	C	1353	5/5	0.99	0.03	25,29,58,59	0
3	SO4	E	1353	5/5	0.99	0.04	35,37,54,58	0
3	SO4	F	1353	5/5	0.99	0.05	20,31,46,51	0
3	SO4	G	1353	5/5	0.99	0.03	24,34,46,62	0
3	SO4	H	1353	5/5	0.99	0.04	38,51,57,63	0
3	SO4	B	1353	5/5	0.99	0.05	19,46,53,63	0
4	CL	D	1354	1/1	0.99	0.06	56,56,56,56	0
4	CL	F	1354	1/1	0.99	0.06	71,71,71,71	0
4	CL	G	1355	1/1	0.99	0.03	41,41,41,41	0
4	CL	H	1354	1/1	0.99	0.03	44,44,44,44	0
4	CL	G	1354	1/1	1.00	0.03	37,37,37,37	0
3	SO4	D	1353	5/5	1.00	0.03	18,23,47,55	0
4	CL	C	1354	1/1	1.00	0.03	49,49,49,49	0
5	ZN	I	1713	1/1	1.00	0.01	38,38,38,38	0
5	ZN	J	1713	1/1	1.00	0.01	40,40,40,40	0
5	ZN	K	1712	1/1	1.00	0.01	30,30,30,30	0
5	ZN	L	1713	1/1	1.00	0.02	36,36,36,36	0
5	ZN	M	1713	1/1	1.00	0.02	43,43,43,43	0
5	ZN	N	1713	1/1	1.00	0.01	34,34,34,34	0
5	ZN	O	1712	1/1	1.00	0.03	57,57,57,57	0
5	ZN	P	1713	1/1	1.00	0.01	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.