



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2023 – 12:32 pm GMT

PDB ID : 7QJJ
Title : X-Ray Structure of a Mn²⁺ soak of EleNRMT in complex with two Nanobodies at 4.6Å
Authors : Ramanadane, K.; Straub, M.S.; Dutzler, R.; Manatschal, C.
Deposited on : 2021-12-16
Resolution : 4.60 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.32.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

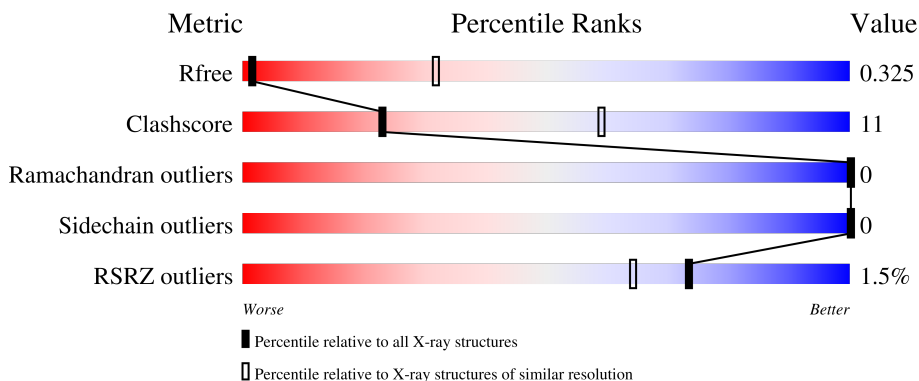
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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.



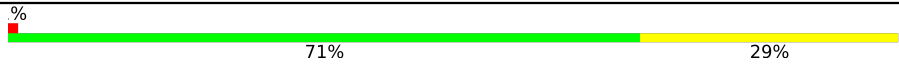
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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	438	 2% 65% 26% 9%
1	E	438	 2% 64% 27% 9%
2	C	117	 85% 14% .
2	F	117	 85% 14% .
3	B	121	 % 71% 29%

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Mol	Chain	Length	Quality of chain
3	G	121	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left representing 71% and a yellow segment on the right representing 29%. A small red square is located at the beginning of the bar, followed by a percentage sign (%).</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9634 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 Divalent metal cation transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	2967	1974	468	505	20	0	0	0
1	E	398	2967	1974	468	505	20	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	GLU	engineered mutation	UNP A0A369N1S1
A	151	SER	ALA	engineered mutation	UNP A0A369N1S1
A	193	GLN	GLU	engineered mutation	UNP A0A369N1S1
A	207	HIS	ARG	engineered mutation	UNP A0A369N1S1
A	244	THR	SER	engineered mutation	UNP A0A369N1S1
A	256	VAL	ILE	engineered mutation	UNP A0A369N1S1
A	275	ALA	SER	engineered mutation	UNP A0A369N1S1
A	366	ILE	VAL	engineered mutation	UNP A0A369N1S1
A	385	ILE	VAL	engineered mutation	UNP A0A369N1S1
A	418	LEU	VAL	engineered mutation	UNP A0A369N1S1
A	429	ALA	VAL	engineered mutation	UNP A0A369N1S1
E	88	GLN	GLU	engineered mutation	UNP A0A369N1S1
E	151	SER	ALA	engineered mutation	UNP A0A369N1S1
E	193	GLN	GLU	engineered mutation	UNP A0A369N1S1
E	207	HIS	ARG	engineered mutation	UNP A0A369N1S1
E	244	THR	SER	engineered mutation	UNP A0A369N1S1
E	256	VAL	ILE	engineered mutation	UNP A0A369N1S1
E	275	ALA	SER	engineered mutation	UNP A0A369N1S1
E	366	ILE	VAL	engineered mutation	UNP A0A369N1S1
E	385	ILE	VAL	engineered mutation	UNP A0A369N1S1
E	418	LEU	VAL	engineered mutation	UNP A0A369N1S1
E	429	ALA	VAL	engineered mutation	UNP A0A369N1S1

- Molecule 2 is a protein called Elen-Nb1-Nb2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	117	Total	C	N	O	S	0	0	0
			908	565	167	171	5			
2	F	117	Total	C	N	O	S	0	0	0
			908	565	167	171	5			

- Molecule 3 is a protein called Elen-Nb1-Nb2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	121	Total	C	N	O	S	0	0	0
			941	591	171	176	3			
3	G	121	Total	C	N	O	S	0	0	0
			941	591	171	176	3			

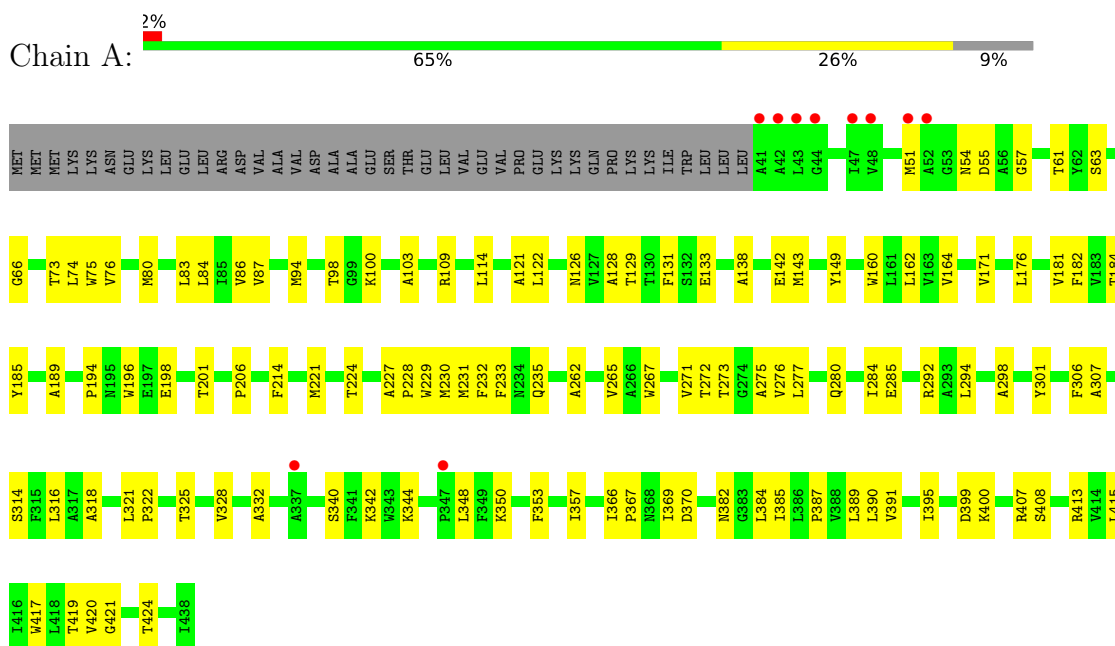
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		

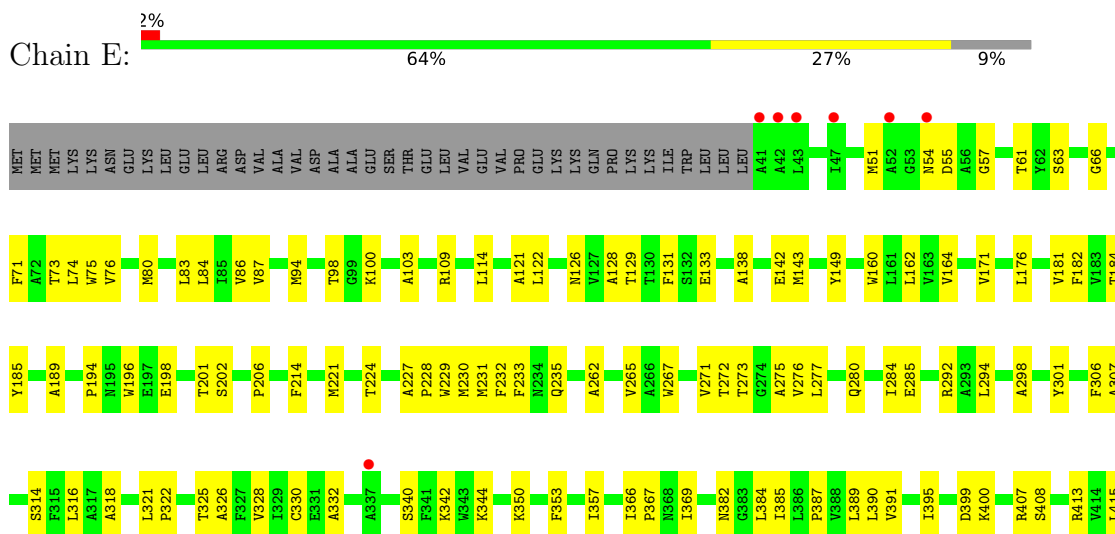
3 Residue-property plots [i](#)

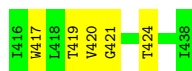
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Divalent metal cation transporter



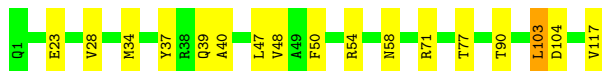
- Molecule 1: Divalent metal cation transporter





- Molecule 2: Elen-Nb1-Nb2

Chain C: 85% 14%



- Molecule 2: Elen-Nb1-Nb2

Chain F: 85% 14%



- Molecule 3: Elen-Nb1-Nb2

Chain B: % 71% 29%



- Molecule 3: Elen-Nb1-Nb2

Chain G: % 71% 29%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.90Å 115.93Å 148.66Å 90.00° 107.59° 90.00°	Depositor
Resolution (Å)	12.00 – 4.60 12.00 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (12.00-4.60) 99.9 (12.00-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 4.52Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.284 , 0.327 0.285 , 0.325	Depositor DCC
R_{free} test set	795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	177.0	Xtrriage
Anisotropy	0.856	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 156.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.177 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9634	wwPDB-VP
Average B, all atoms (Å ²)	270.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: 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	0.26	0/3030	0.46	0/4135
1	E	0.26	0/3030	0.46	0/4135
2	C	0.26	0/925	0.58	1/1248 (0.1%)
2	F	0.26	0/925	0.58	1/1248 (0.1%)
3	B	0.26	0/963	0.58	0/1305
3	G	0.27	0/963	0.58	0/1305
All	All	0.26	0/9836	0.51	2/13376 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	103	LEU	CA-CB-CG	5.62	128.23	115.30
2	C	103	LEU	CA-CB-CG	5.59	128.16	115.30

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	2967	0	3125	72	8
1	E	2967	0	3125	72	8
2	C	908	0	896	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	908	0	896	13	0
3	B	941	0	906	28	0
3	G	941	0	906	28	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
All	All	9634	0	9854	222	8

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 11.

The worst 5 of 222 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)
3:G:34:LEU:HB2	3:G:79:VAL:HG21	1.72	0.71
3:B:34:LEU:HB2	3:B:79:VAL:HG21	1.72	0.71
1:E:273:THR:HG23	1:E:277:LEU:HD12	1.75	0.68
1:A:273:THR:HG23	1:A:277:LEU:HD12	1.75	0.66
1:E:340:SER:HB2	1:E:344:LYS:HB2	1.77	0.66

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:CE	1:E:344:LYS:CE[2_444]	1.11	1.09
1:A:342:LYS:CB	1:E:342:LYS:O[2_444]	1.17	1.03
1:A:342:LYS:O	1:E:342:LYS:CB[2_444]	1.20	1.00
1:A:342:LYS:O	1:E:342:LYS:CG[2_444]	1.73	0.47
1:A:342:LYS:CG	1:E:342:LYS:O[2_444]	1.87	0.33

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	396/438 (90%)	375 (95%)	21 (5%)	0	100	100
1	E	396/438 (90%)	375 (95%)	21 (5%)	0	100	100
2	C	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
2	F	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
3	B	119/121 (98%)	100 (84%)	19 (16%)	0	100	100
3	G	119/121 (98%)	100 (84%)	19 (16%)	0	100	100
All	All	1260/1352 (93%)	1160 (92%)	100 (8%)	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	308/345 (89%)	308 (100%)	0	100	100
1	E	308/345 (89%)	308 (100%)	0	100	100
2	C	96/96 (100%)	96 (100%)	0	100	100
2	F	96/96 (100%)	96 (100%)	0	100	100
3	B	95/95 (100%)	95 (100%)	0	100	100
3	G	95/95 (100%)	95 (100%)	0	100	100
All	All	998/1072 (93%)	998 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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	398/438 (90%)	-0.01	10 (2%) 57 48	169, 257, 398, 745	0
1	E	398/438 (90%)	-0.02	7 (1%) 68 60	189, 267, 392, 694	0
2	C	117/117 (100%)	-0.19	0 100 100	198, 265, 313, 368	0
2	F	117/117 (100%)	-0.13	0 100 100	185, 249, 301, 340	0
3	B	121/121 (100%)	-0.20	1 (0%) 86 79	201, 256, 322, 377	0
3	G	121/121 (100%)	-0.22	1 (0%) 86 79	201, 268, 328, 393	0
All	All	1272/1352 (94%)	-0.08	19 (1%) 73 64	169, 260, 369, 745	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	ALA	6.2
1	A	41	ALA	5.4
1	E	43	LEU	4.6
1	E	41	ALA	4.5
1	A	48	VAL	4.1

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 monosaccharides 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
4	MN	E	501	1/1	0.95	0.22	200,200,200,200	0
4	MN	A	501	1/1	0.98	0.22	182,182,182,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.