



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2NP3 / pdb_00002np3
Title : Crystal structure of TetR-family regulator (SCO0857) from *Streptomyces coelicolor* A3.
Authors : Koclega, K.D.; Xu, X.; Chruszcz, M.; Gu, J.; Cymborowski, M.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Minor, W.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-10-26
Resolution : 2.35 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
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

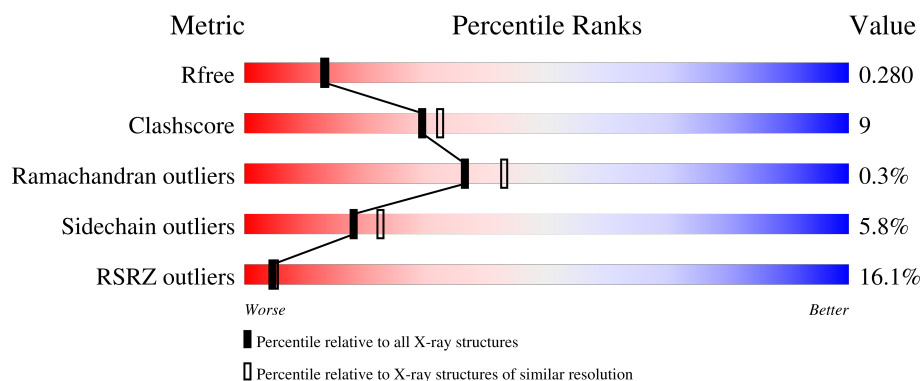
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 ≥ 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	212	16% 53% 14% 33%
1	B	212	8% 65% 20% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2395 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 Putative TetR-family regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	Se	0	2	1
			1022	639	191	184	1	7			
1	B	180	Total	C	N	O	S	Se	0	2	0
			1346	839	249	250	1	7			

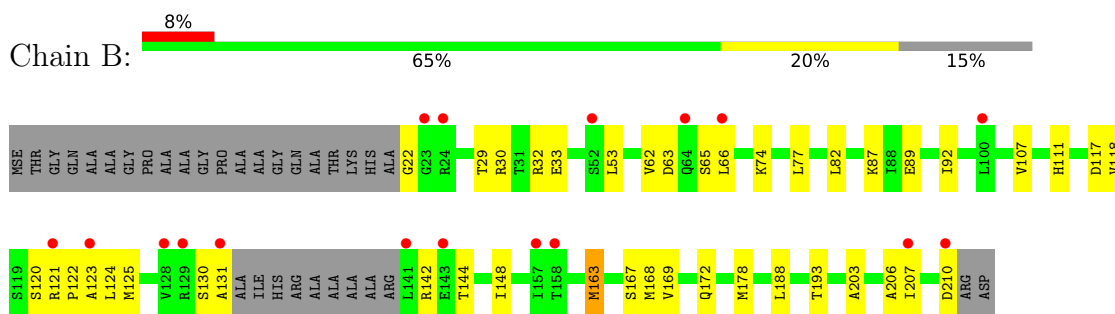
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9RCV4
A	125	MSE	MET	modified residue	UNP Q9RCV4
A	127	MSE	MET	modified residue	UNP Q9RCV4
A	163	MSE	MET	modified residue	UNP Q9RCV4
A	168	MSE	MET	modified residue	UNP Q9RCV4
A	178	MSE	MET	modified residue	UNP Q9RCV4
A	179	MSE	MET	modified residue	UNP Q9RCV4
B	1	MSE	MET	modified residue	UNP Q9RCV4
B	125	MSE	MET	modified residue	UNP Q9RCV4
B	127	MSE	MET	modified residue	UNP Q9RCV4
B	163	MSE	MET	modified residue	UNP Q9RCV4
B	168	MSE	MET	modified residue	UNP Q9RCV4
B	178	MSE	MET	modified residue	UNP Q9RCV4
B	179	MSE	MET	modified residue	UNP Q9RCV4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	23	Total	O	0	0
			23	23		

- Molecule 1: Putative TetR-family regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.43Å 92.77Å 93.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.59 – 2.35 41.59 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.59-2.35) 99.0 (41.59-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	18.20 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.264 0.239 , 0.280	Depositor DCC
R_{free} test set	917 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2395	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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](#)

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	1.13	1/1030 (0.1%)	1.21	4/1382 (0.3%)
1	B	1.28	4/1358 (0.3%)	1.23	3/1824 (0.2%)
All	All	1.22	5/2388 (0.2%)	1.22	7/3206 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	MSE	SE-CE	7.71	2.18	1.95
1	B	123	ALA	CA-C	5.55	1.59	1.52
1	B	123	ALA	CA-CB	5.33	1.61	1.53
1	A	127	MSE	SE-CE	5.20	2.11	1.95
1	B	167	SER	CA-C	5.14	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	GLY	N-CA-C	6.96	119.94	111.93
1	B	87	LYS	N-CA-C	6.58	118.53	111.36
1	B	77	LEU	N-CA-C	5.96	118.27	111.11
1	A	158	THR	N-CA-C	5.94	121.41	114.04
1	B	118	VAL	N-CA-C	5.50	116.22	110.62
1	A	107	VAL	N-CA-C	5.36	116.08	110.62
1	A	207	ILE	N-CA-C	-5.05	105.92	110.82

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	1022	0	1025	15	0
1	B	1346	0	1360	27	0
2	A	4	0	0	0	0
2	B	23	0	0	0	0
All	All	2395	0	2385	41	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 9.

All (41) 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:B:163:MSE:CE	1:B:163:MSE:SE	2.18	1.40
1:B:168:MSE:CE	1:B:207:ILE:HD12	1.66	1.25
1:B:168:MSE:HE2	1:B:207:ILE:HD12	1.14	1.04
1:A:179:MSE:HE2	1:A:185:LEU:HB2	1.40	1.04
1:A:179:MSE:CE	1:A:185:LEU:HB2	1.93	0.99
1:B:168:MSE:CE	1:B:207:ILE:CD1	2.41	0.96
1:B:168:MSE:HE2	1:B:207:ILE:CD1	2.05	0.76
1:B:168:MSE:HE1	1:B:207:ILE:HD12	1.67	0.74
1:A:179:MSE:HE2	1:A:185:LEU:CB	2.19	0.70
1:B:62:VAL:HB	1:B:66:LEU:HD13	1.76	0.67
1:B:130:SER:O	1:B:131:ALA:O	2.16	0.64
1:B:62:VAL:HB	1:B:66:LEU:CD1	2.30	0.62
1:B:168:MSE:HE1	1:B:207:ILE:CD1	2.26	0.59
1:A:87:LYS:NZ	1:A:117:ASP:OD2	2.38	0.56
1:B:130:SER:O	1:B:131:ALA:C	2.48	0.56
1:B:22:GLY:CA	1:B:32:ARG:HD2	2.36	0.56
1:A:119:SER:HA	1:A:125:MSE:SE	2.56	0.56
1:B:22:GLY:HA3	1:B:29:THR:HA	1.87	0.55
1:B:121:ARG:HD2	1:B:124:LEU:HD12	1.90	0.53
1:B:169:VAL:HA	1:B:172:GLN:HE21	1.74	0.52
1:B:142:ARG:HD3	1:B:178[A]:MSE:SE	2.60	0.51
1:A:36:LEU:O	1:A:40:ARG:HG3	2.11	0.51
1:A:88:ILE:HG13	1:A:114:VAL:HG11	1.95	0.48
1:A:207:ILE:HD11	1:B:203:ALA:HB2	1.95	0.48
1:B:92:ILE:HD11	1:B:111:HIS:HB2	1.95	0.48
1:B:63:ASP:OD1	1:B:63:ASP:C	2.58	0.47
1:A:168:MSE:O	1:A:172:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PHE:O	1:A:82:LEU:HB2	2.15	0.46
1:A:84:LEU:HD13	1:A:118:VAL:HG21	1.98	0.45
1:B:22:GLY:HA2	1:B:32:ARG:HD2	1.98	0.45
1:A:179:MSE:CE	1:A:185:LEU:CB	2.82	0.45
1:A:179:MSE:HE2	1:A:185:LEU:HD22	1.98	0.45
1:B:53:LEU:HD21	1:B:74:LYS:HA	1.99	0.44
1:B:29:THR:O	1:B:33:GLU:HG3	2.18	0.44
1:B:206:ALA:O	1:B:210:ASP:HB2	2.19	0.42
1:B:144:THR:HG22	1:B:148:ILE:HD12	2.01	0.42
1:A:84:LEU:HB3	1:A:85:PRO:HD3	2.02	0.42
1:B:121:ARG:HA	1:B:122:PRO:HD3	1.94	0.41
1:B:22:GLY:HA2	1:B:32:ARG:CD	2.51	0.41
1:B:117:ASP:O	1:B:120:SER:HB2	2.21	0.41
1:A:121:ARG:HD2	1:A:124:LEU:HD12	2.03	0.41

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	139/212 (66%)	132 (95%)	6 (4%)	1 (1%)	18	20
1	B	178/212 (84%)	170 (96%)	8 (4%)	0	100	100
All	All	317/424 (75%)	302 (95%)	14 (4%)	1 (0%)	36	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	VAL

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	95/144 (66%)	89 (94%)	6 (6%)	16	19
1	B	132/144 (92%)	123 (93%)	9 (7%)	14	16
All	All	227/288 (79%)	212 (93%)	15 (7%)	18	17

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	164	LEU
1	A	178[A]	MSE
1	A	178[B]	MSE
1	A	188	LEU
1	A	209	THR
1	B	30[A]	ARG
1	B	30[B]	ARG
1	B	65	SER
1	B	82	LEU
1	B	89	GLU
1	B	107	VAL
1	B	125	MSE
1	B	188	LEU
1	B	193	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	111	HIS
1	B	68	HIS
1	B	69	HIS
1	B	97	GLN

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](#)

There are no ligands in this entry.

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	137/212 (64%)	1.49	33 (24%) 2 1	36, 54, 82, 86	1 (0%)
1	B	174/212 (82%)	0.86	17 (9%) 13 15	24, 47, 65, 80	1 (0%)
All	All	311/424 (73%)	1.14	50 (16%) 4 5	24, 51, 73, 86	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	VAL	8.8
1	A	78	PHE	8.2
1	B	123	ALA	6.0
1	A	130	SER	5.6
1	A	71	TYR	5.5
1	A	77	LEU	5.0
1	A	138	ALA	4.5
1	A	155	GLY	4.4
1	A	82	LEU	4.0
1	A	74	LYS	3.8
1	A	75	GLU	3.7
1	B	157	ILE	3.4
1	A	126	THR	3.2
1	A	123	ALA	3.2
1	A	139	ALA	3.2
1	B	141	LEU	3.1
1	A	211	ARG	3.1
1	A	35	ILE	3.1
1	A	210	ASP	3.0
1	B	23	GLY	3.0
1	B	210	ASP	3.0
1	A	114	VAL	2.9
1	A	156	VAL	2.9
1	A	79	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	72	GLY	2.8
1	A	192	ASP	2.8
1	A	76	ASN	2.7
1	B	131	ALA	2.7
1	B	128	VAL	2.7
1	A	37	THR	2.6
1	A	140	ARG	2.6
1	B	64	GLN	2.4
1	B	158	THR	2.4
1	A	42	CYS	2.4
1	A	184	HIS	2.4
1	B	52	SER	2.3
1	A	36	LEU	2.3
1	A	94	ALA	2.3
1	B	143	GLU	2.3
1	B	207	ILE	2.3
1	A	43	PHE	2.2
1	A	207	ILE	2.2
1	B	24	ARG	2.1
1	A	73	THR	2.1
1	B	66	LEU	2.1
1	A	80	GLN	2.1
1	B	100	LEU	2.0
1	A	99	GLY	2.0
1	B	121	ARG	2.0
1	B	129	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.