wwPDB X-ray Structure Validation Summary Report (i)

Sep 20, 2023 – 07:36 AM EDT

PDB ID	:	5JTG
Title	:	Crystal structure of Thermotoga maritima mutant D89K/D253K
Authors	:	Kowatz, T.; Maguire, M.
Deposited on	:	2016-05-09
Resolution	:	3.05 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 (i) 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 (i)) were used in the production of this report:

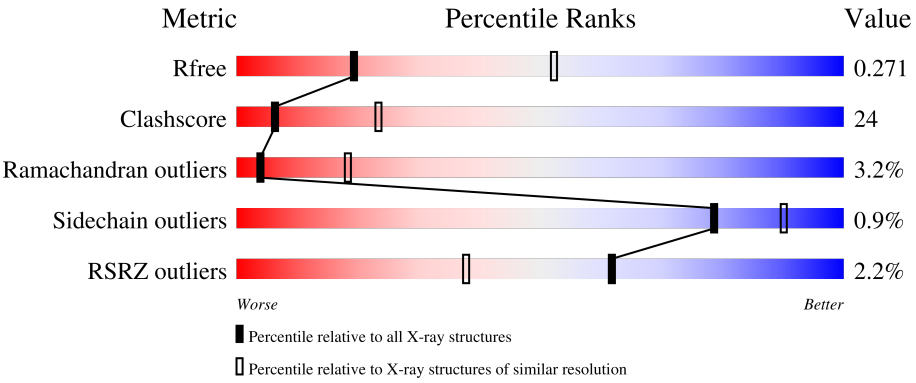
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 <=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	373	% 53% 29% • 13%
1	B	373	4% 50% 33% • 14%
1	C	373	3% 52% 31% • 14%
1	D	373	% 53% 31% • 13%
1	E	373	% 54% 29% • 14%

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
2	MG	A	401	-	-	-	X
2	MG	B	401	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13344 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 Cobalt/magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2678	1746	436	488	8			
1	B	321	Total	C	N	O	S	0	0	0
			2662	1734	434	486	8			
1	C	320	Total	C	N	O	S	0	0	0
			2657	1732	433	484	8			
1	D	323	Total	C	N	O	S	0	0	0
			2678	1746	436	488	8			
1	E	320	Total	C	N	O	S	0	0	0
			2660	1734	433	485	8			

There are 125 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q9WZ31
A	-20	GLY	-	expression tag	UNP Q9WZ31
A	-19	SER	-	expression tag	UNP Q9WZ31
A	-18	SER	-	expression tag	UNP Q9WZ31
A	-17	HIS	-	expression tag	UNP Q9WZ31
A	-16	HIS	-	expression tag	UNP Q9WZ31
A	-15	HIS	-	expression tag	UNP Q9WZ31
A	-14	HIS	-	expression tag	UNP Q9WZ31
A	-13	HIS	-	expression tag	UNP Q9WZ31
A	-12	HIS	-	expression tag	UNP Q9WZ31
A	-11	SER	-	expression tag	UNP Q9WZ31
A	-10	SER	-	expression tag	UNP Q9WZ31
A	-9	GLY	-	expression tag	UNP Q9WZ31
A	-8	ARG	-	expression tag	UNP Q9WZ31
A	-7	GLU	-	expression tag	UNP Q9WZ31
A	-6	ASN	-	expression tag	UNP Q9WZ31
A	-5	LEU	-	expression tag	UNP Q9WZ31
A	-4	TYR	-	expression tag	UNP Q9WZ31
A	-3	PHE	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	expression tag	UNP Q9WZ31
A	-1	GLY	-	expression tag	UNP Q9WZ31
A	0	HIS	-	expression tag	UNP Q9WZ31
A	1	VAL	-	expression tag	UNP Q9WZ31
A	89	LYS	ASP	engineered mutation	UNP Q9WZ31
A	253	LYS	ASP	engineered mutation	UNP Q9WZ31
B	-21	MET	-	expression tag	UNP Q9WZ31
B	-20	GLY	-	expression tag	UNP Q9WZ31
B	-19	SER	-	expression tag	UNP Q9WZ31
B	-18	SER	-	expression tag	UNP Q9WZ31
B	-17	HIS	-	expression tag	UNP Q9WZ31
B	-16	HIS	-	expression tag	UNP Q9WZ31
B	-15	HIS	-	expression tag	UNP Q9WZ31
B	-14	HIS	-	expression tag	UNP Q9WZ31
B	-13	HIS	-	expression tag	UNP Q9WZ31
B	-12	HIS	-	expression tag	UNP Q9WZ31
B	-11	SER	-	expression tag	UNP Q9WZ31
B	-10	SER	-	expression tag	UNP Q9WZ31
B	-9	GLY	-	expression tag	UNP Q9WZ31
B	-8	ARG	-	expression tag	UNP Q9WZ31
B	-7	GLU	-	expression tag	UNP Q9WZ31
B	-6	ASN	-	expression tag	UNP Q9WZ31
B	-5	LEU	-	expression tag	UNP Q9WZ31
B	-4	TYR	-	expression tag	UNP Q9WZ31
B	-3	PHE	-	expression tag	UNP Q9WZ31
B	-2	GLN	-	expression tag	UNP Q9WZ31
B	-1	GLY	-	expression tag	UNP Q9WZ31
B	0	HIS	-	expression tag	UNP Q9WZ31
B	1	VAL	-	expression tag	UNP Q9WZ31
B	89	LYS	ASP	engineered mutation	UNP Q9WZ31
B	253	LYS	ASP	engineered mutation	UNP Q9WZ31
C	-21	MET	-	expression tag	UNP Q9WZ31
C	-20	GLY	-	expression tag	UNP Q9WZ31
C	-19	SER	-	expression tag	UNP Q9WZ31
C	-18	SER	-	expression tag	UNP Q9WZ31
C	-17	HIS	-	expression tag	UNP Q9WZ31
C	-16	HIS	-	expression tag	UNP Q9WZ31
C	-15	HIS	-	expression tag	UNP Q9WZ31
C	-14	HIS	-	expression tag	UNP Q9WZ31
C	-13	HIS	-	expression tag	UNP Q9WZ31
C	-12	HIS	-	expression tag	UNP Q9WZ31
C	-11	SER	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	SER	-	expression tag	UNP Q9WZ31
C	-9	GLY	-	expression tag	UNP Q9WZ31
C	-8	ARG	-	expression tag	UNP Q9WZ31
C	-7	GLU	-	expression tag	UNP Q9WZ31
C	-6	ASN	-	expression tag	UNP Q9WZ31
C	-5	LEU	-	expression tag	UNP Q9WZ31
C	-4	TYR	-	expression tag	UNP Q9WZ31
C	-3	PHE	-	expression tag	UNP Q9WZ31
C	-2	GLN	-	expression tag	UNP Q9WZ31
C	-1	GLY	-	expression tag	UNP Q9WZ31
C	0	HIS	-	expression tag	UNP Q9WZ31
C	1	VAL	-	expression tag	UNP Q9WZ31
C	89	LYS	ASP	engineered mutation	UNP Q9WZ31
C	253	LYS	ASP	engineered mutation	UNP Q9WZ31
D	-21	MET	-	expression tag	UNP Q9WZ31
D	-20	GLY	-	expression tag	UNP Q9WZ31
D	-19	SER	-	expression tag	UNP Q9WZ31
D	-18	SER	-	expression tag	UNP Q9WZ31
D	-17	HIS	-	expression tag	UNP Q9WZ31
D	-16	HIS	-	expression tag	UNP Q9WZ31
D	-15	HIS	-	expression tag	UNP Q9WZ31
D	-14	HIS	-	expression tag	UNP Q9WZ31
D	-13	HIS	-	expression tag	UNP Q9WZ31
D	-12	HIS	-	expression tag	UNP Q9WZ31
D	-11	SER	-	expression tag	UNP Q9WZ31
D	-10	SER	-	expression tag	UNP Q9WZ31
D	-9	GLY	-	expression tag	UNP Q9WZ31
D	-8	ARG	-	expression tag	UNP Q9WZ31
D	-7	GLU	-	expression tag	UNP Q9WZ31
D	-6	ASN	-	expression tag	UNP Q9WZ31
D	-5	LEU	-	expression tag	UNP Q9WZ31
D	-4	TYR	-	expression tag	UNP Q9WZ31
D	-3	PHE	-	expression tag	UNP Q9WZ31
D	-2	GLN	-	expression tag	UNP Q9WZ31
D	-1	GLY	-	expression tag	UNP Q9WZ31
D	0	HIS	-	expression tag	UNP Q9WZ31
D	1	VAL	-	expression tag	UNP Q9WZ31
D	89	LYS	ASP	engineered mutation	UNP Q9WZ31
D	253	LYS	ASP	engineered mutation	UNP Q9WZ31
E	-21	MET	-	expression tag	UNP Q9WZ31
E	-20	GLY	-	expression tag	UNP Q9WZ31
E	-19	SER	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	SER	-	expression tag	UNP Q9WZ31
E	-17	HIS	-	expression tag	UNP Q9WZ31
E	-16	HIS	-	expression tag	UNP Q9WZ31
E	-15	HIS	-	expression tag	UNP Q9WZ31
E	-14	HIS	-	expression tag	UNP Q9WZ31
E	-13	HIS	-	expression tag	UNP Q9WZ31
E	-12	HIS	-	expression tag	UNP Q9WZ31
E	-11	SER	-	expression tag	UNP Q9WZ31
E	-10	SER	-	expression tag	UNP Q9WZ31
E	-9	GLY	-	expression tag	UNP Q9WZ31
E	-8	ARG	-	expression tag	UNP Q9WZ31
E	-7	GLU	-	expression tag	UNP Q9WZ31
E	-6	ASN	-	expression tag	UNP Q9WZ31
E	-5	LEU	-	expression tag	UNP Q9WZ31
E	-4	TYR	-	expression tag	UNP Q9WZ31
E	-3	PHE	-	expression tag	UNP Q9WZ31
E	-2	GLN	-	expression tag	UNP Q9WZ31
E	-1	GLY	-	expression tag	UNP Q9WZ31
E	0	HIS	-	expression tag	UNP Q9WZ31
E	1	VAL	-	expression tag	UNP Q9WZ31
E	89	LYS	ASP	engineered mutation	UNP Q9WZ31
E	253	LYS	ASP	engineered mutation	UNP Q9WZ31

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0

- Molecule 3 is water.

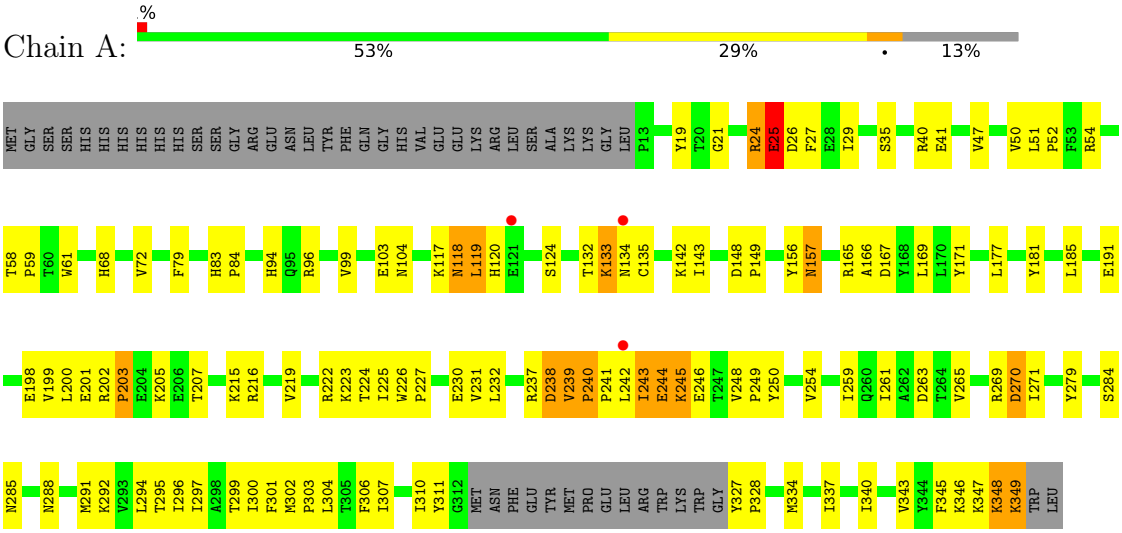
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 1 1	0	0
3	D	4	Total O 4 4	0	0

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.

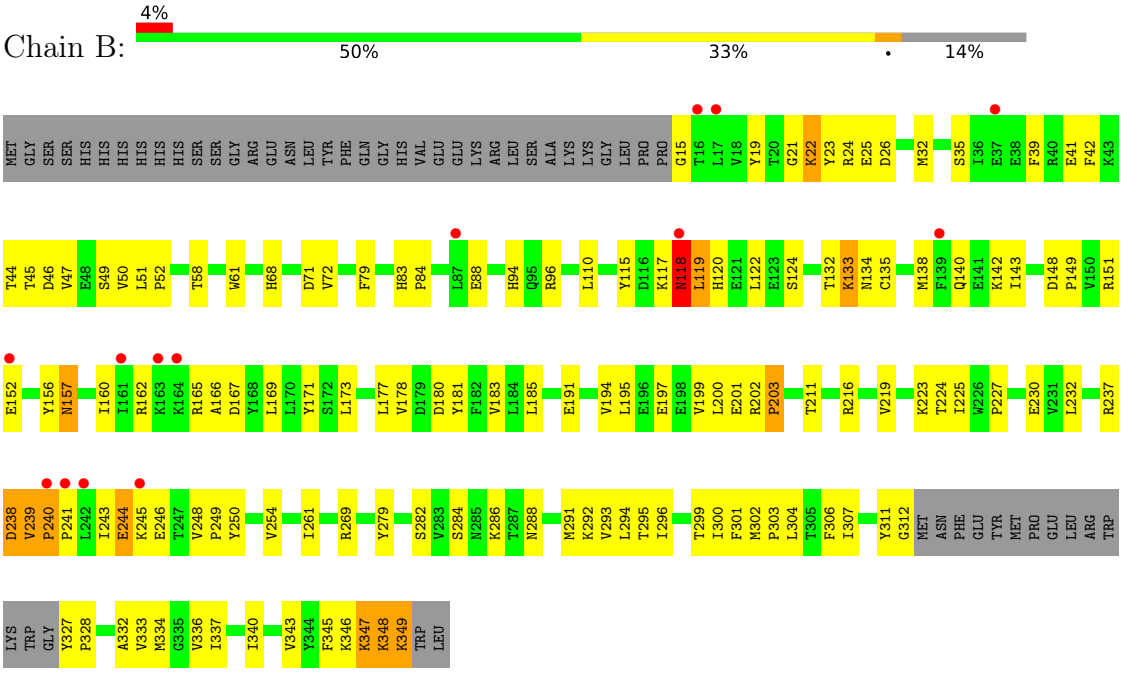
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain A:



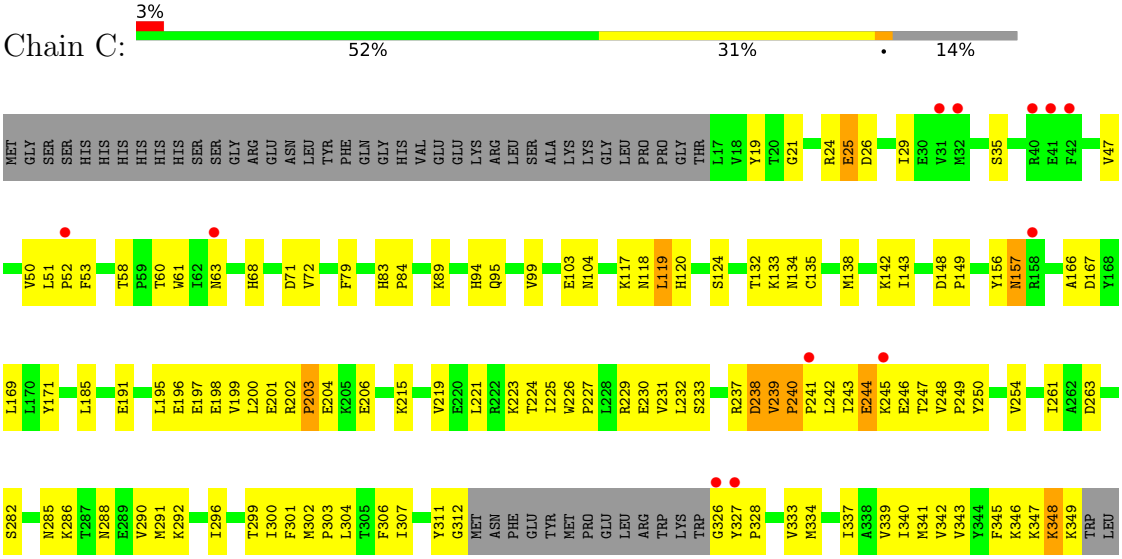
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain B:



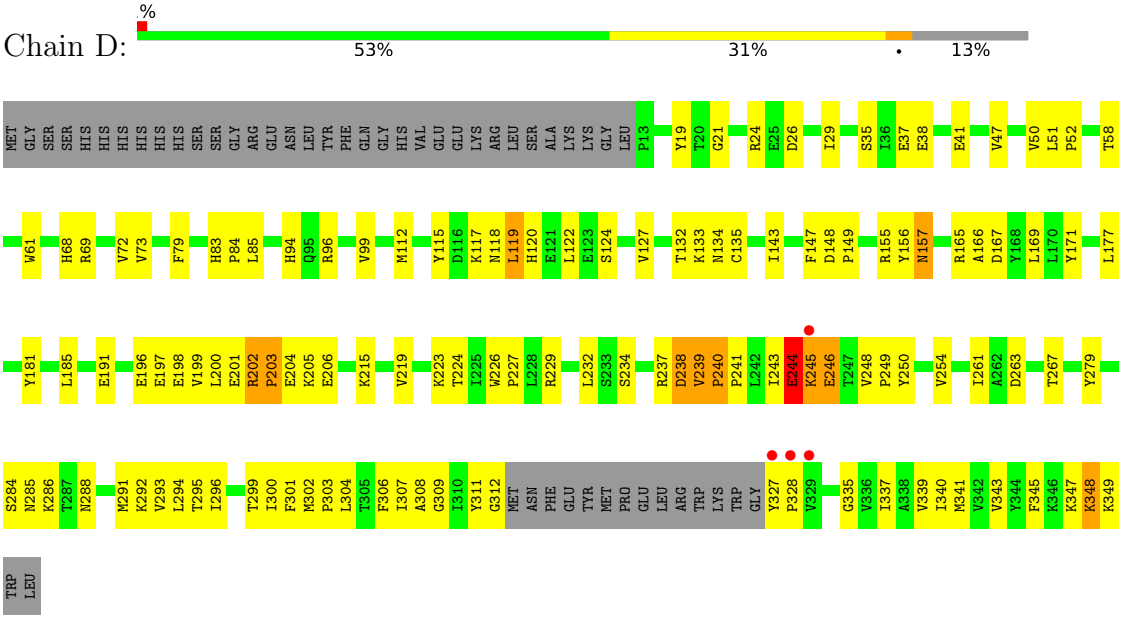
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain C:



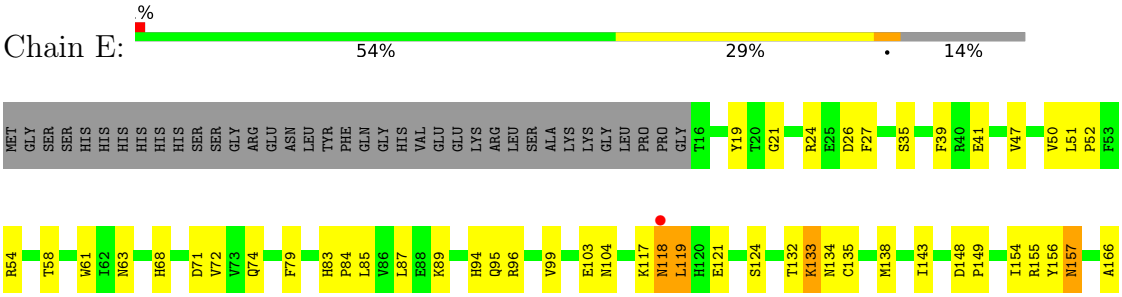
• Molecule 1: Cobalt/magnesium transport protein CorA

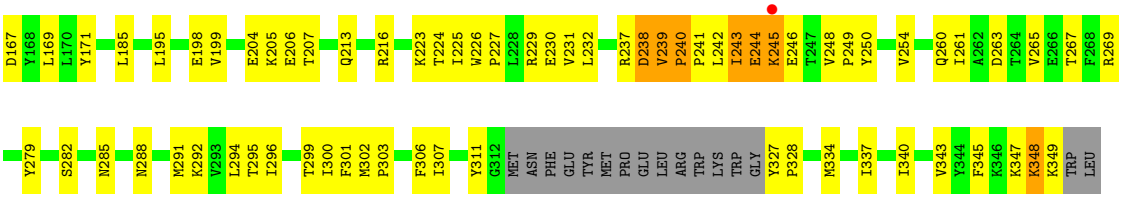
Chain D:



• Molecule 1: Cobalt/magnesium transport protein CorA

Chain E:




D167 Y168 L169 L170 Y171 L185 L195 E198 V199 E204 K205 E206 T207 Q213 R216 K223 T224 I225 W226 P227 L228 R229 E230 V231 L232 R237 D238 V239 P240 P241 L242 I243 E244 K245 E246 T247 V248 P249 Y250 V254 Q260 I261 A262 D263 T264 V265 E266 T267 F268 R269
Y279 S282 N285 N288 M291 K292 V293 L294 T295 I296 T299 I300 F301 M302 P303 F306 I307 Y311 G312 MET ASN PHE GLU TYR MET PRO GLU LEU ARG TRP LYS TRP GLY Y327 P328 M334 I337 I340 V343 Y344 F345 K346 K347 K348 K349 TRP LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.12Å 104.49Å 122.82Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	47.77 – 3.05 47.77 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.77-3.05) 99.3 (47.77-3.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.246 , 0.291 0.229 , 0.271	Depositor DCC
R_{free} test set	2823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	102.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 69.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13344	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG

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	0.45	0/2734	0.58	0/3704
1	B	0.42	0/2716	0.57	0/3678
1	C	0.43	0/2711	0.58	0/3671
1	D	0.54	3/2734 (0.1%)	0.59	1/3704 (0.0%)
1	E	0.47	0/2714	0.60	0/3676
All	All	0.47	3/13609 (0.0%)	0.58	1/18433 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
1	C	0	4
1	D	0	4
1	E	0	3
All	All	0	24

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	312	GLY	C-O	8.66	1.37	1.23
1	D	312	GLY	N-CA	7.27	1.56	1.46
1	D	312	GLY	CA-C	7.11	1.63	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	312	GLY	N-CA-C	5.41	126.63	113.10

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	LEU	Peptide
1	A	203	PRO	Peptide
1	A	24	ARG	Peptide
1	A	25	GLU	Peptide
1	A	94	HIS	Peptide

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	2678	0	2742	159	0
1	B	2662	0	2720	149	2
1	C	2657	0	2720	131	2
1	D	2678	0	2742	152	0
1	E	2660	0	2724	134	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	E	2	0	0	0	0
3	B	1	0	0	0	0
3	D	4	0	0	0	0
All	All	13344	0	13648	654	2

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 24.

The worst 5 of 654 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:26:ASP:OD2	1:B:143:ILE:HG22	1.39	1.22
1:B:203:PRO:HG2	1:B:286:LYS:HE3	1.27	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:CD	1:A:245:LYS:H	1.57	1.06
1:C:244:GLU:O	1:C:246:GLU:N	1.90	1.05
1:A:244:GLU:O	1:A:246:GLU:N	1.90	1.04

All (2) 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:B:156:TYR:OH	1:C:117:LYS:CE[2_545]	1.90	0.30
1:B:156:TYR:OH	1:C:117:LYS:NZ[2_545]	2.19	0.01

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	319/373 (86%)	280 (88%)	28 (9%)	11 (3%)	3	17
1	B	317/373 (85%)	281 (89%)	27 (8%)	9 (3%)	5	21
1	C	316/373 (85%)	280 (89%)	26 (8%)	10 (3%)	4	18
1	D	319/373 (86%)	280 (88%)	28 (9%)	11 (3%)	3	17
1	E	316/373 (85%)	281 (89%)	26 (8%)	9 (3%)	5	21
All	All	1587/1865 (85%)	1402 (88%)	135 (8%)	50 (3%)	4	18

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	118	ASN
1	A	240	PRO
1	A	244	GLU
1	A	245	LYS

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	305/349 (87%)	302 (99%)	3 (1%)	76 89
1	B	302/349 (86%)	296 (98%)	6 (2%)	55 78
1	C	302/349 (86%)	300 (99%)	2 (1%)	84 92
1	D	305/349 (87%)	303 (99%)	2 (1%)	84 92
1	E	303/349 (87%)	302 (100%)	1 (0%)	92 96
All	All	1517/1745 (87%)	1503 (99%)	14 (1%)	78 90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	284	SER
1	B	349	LYS
1	E	124	SER
1	D	124	SER
1	D	284	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	ASN
1	E	95	GLN
1	C	104	ASN
1	E	288	ASN
1	D	288	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 monosaccharides 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^{th} 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	323/373 (86%)	-0.27	3 (0%)	84	66	79, 115, 170, 191	0
1	B	321/373 (86%)	0.01	14 (4%)	34	16	80, 144, 207, 261	0
1	C	320/373 (85%)	-0.03	12 (3%)	40	20	75, 136, 192, 220	0
1	D	323/373 (86%)	-0.26	4 (1%)	79	58	69, 109, 181, 200	0
1	E	320/373 (85%)	-0.31	2 (0%)	89	76	71, 107, 175, 202	0
All	All	1607/1865 (86%)	-0.17	35 (2%)	62	38	69, 119, 187, 261	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	LYS	6.5
1	C	41	GLU	5.5
1	C	31	VAL	4.8
1	C	42	PHE	4.6
1	B	242	LEU	4.3

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^{th} 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
2	MG	B	401	1/1	0.70	0.57	110,110,110,110	0
2	MG	A	401	1/1	0.77	0.74	105,105,105,105	0
2	MG	E	401	1/1	0.85	0.24	99,99,99,99	0
2	MG	E	402	1/1	0.87	0.11	102,102,102,102	0

6.5 Other polymers (i)

There are no such residues in this entry.