WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 03:56 AM EDT

PDB ID	:	1TWY
Title	:	Crystal structure of an ABC-type phosphate transport receptor from Vibrio cholerae
Authors	:	Ramagopal, U.A.; Patskovsky, Y.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-07-01
Resolution	:	1.65 Å(reported)

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

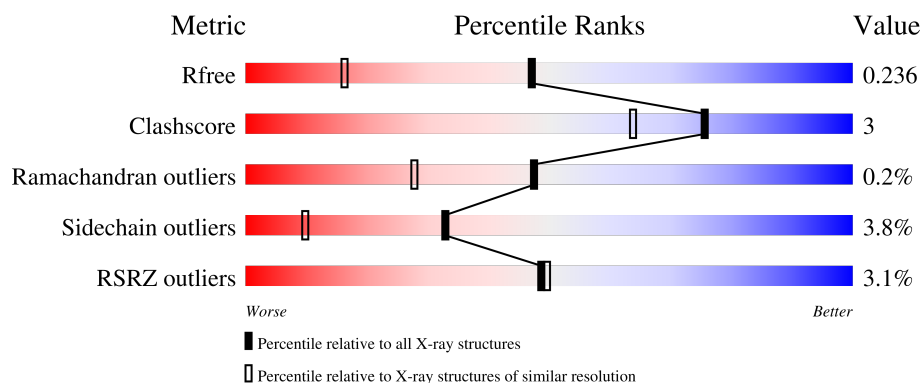|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.65 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		3.8%
RSRZ outliers		3.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	290	3% — 77% · 8% · 14%
1	B	290	3% — 75% · 9% · 16%
1	C	290	3% — 71% · 12% · 14%
1	D	290	3% — 78% · 8% · 14%
1	E	290	2% — 76% · 8% · 14%

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Mol	Chain	Length	Quality of chain
1	F	290	2% ▮ 72% 11% • 15%
1	G	290	3% ▮ 74% 11% • 14%
1	H	290	2% ▮ 73% 11% • 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	PO4	C	1507	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16805 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 ABC transporter, periplasmic substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total 1919	C 1208	N 324	O 381	Se 6	0	1	0
1	B	244	Total 1890	C 1191	N 318	O 375	Se 6	0	2	0
1	C	249	Total 1937	C 1219	N 327	O 385	Se 6	0	5	0
1	D	249	Total 1918	C 1208	N 324	O 380	Se 6	0	0	0
1	E	248	Total 1917	C 1207	N 324	O 380	Se 6	0	2	0
1	F	247	Total 1910	C 1201	N 323	O 380	Se 6	0	3	0
1	G	249	Total 1924	C 1211	N 324	O 383	Se 6	0	2	0
1	H	249	Total 1937	C 1219	N 328	O 384	Se 6	0	5	0

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	GB 15601562
A	2	SER	-	cloning artifact	GB 15601562
A	3	LEU	-	cloning artifact	GB 15601562
A	42	MSE	MET	modified residue	GB 15601562
A	81	MSE	MET	modified residue	GB 15601562
A	163	MSE	MET	modified residue	GB 15601562
A	189	MSE	MET	modified residue	GB 15601562
A	190	MSE	MET	modified residue	GB 15601562
A	275	MSE	MET	modified residue	GB 15601562
A	281	GLU	-	cloning artifact	GB 15601562
A	282	GLY	-	cloning artifact	GB 15601562
A	283	GLY	-	cloning artifact	GB 15601562
A	284	SER	-	cloning artifact	GB 15601562

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Chain	Residue	Modelled	Actual	Comment	Reference
A	285	HIS	-	cloning artifact	GB 15601562
A	286	HIS	-	cloning artifact	GB 15601562
A	287	HIS	-	cloning artifact	GB 15601562
A	288	HIS	-	cloning artifact	GB 15601562
A	289	HIS	-	cloning artifact	GB 15601562
A	290	HIS	-	cloning artifact	GB 15601562
B	1	MET	-	cloning artifact	GB 15601562
B	2	SER	-	cloning artifact	GB 15601562
B	3	LEU	-	cloning artifact	GB 15601562
B	42	MSE	MET	modified residue	GB 15601562
B	81	MSE	MET	modified residue	GB 15601562
B	163	MSE	MET	modified residue	GB 15601562
B	189	MSE	MET	modified residue	GB 15601562
B	190	MSE	MET	modified residue	GB 15601562
B	275	MSE	MET	modified residue	GB 15601562
B	281	GLU	-	cloning artifact	GB 15601562
B	282	GLY	-	cloning artifact	GB 15601562
B	283	GLY	-	cloning artifact	GB 15601562
B	284	SER	-	cloning artifact	GB 15601562
B	285	HIS	-	cloning artifact	GB 15601562
B	286	HIS	-	cloning artifact	GB 15601562
B	287	HIS	-	cloning artifact	GB 15601562
B	288	HIS	-	cloning artifact	GB 15601562
B	289	HIS	-	cloning artifact	GB 15601562
B	290	HIS	-	cloning artifact	GB 15601562
C	1	MET	-	cloning artifact	GB 15601562
C	2	SER	-	cloning artifact	GB 15601562
C	3	LEU	-	cloning artifact	GB 15601562
C	42	MSE	MET	modified residue	GB 15601562
C	81	MSE	MET	modified residue	GB 15601562
C	163	MSE	MET	modified residue	GB 15601562
C	189	MSE	MET	modified residue	GB 15601562
C	190	MSE	MET	modified residue	GB 15601562
C	275	MSE	MET	modified residue	GB 15601562
C	281	GLU	-	cloning artifact	GB 15601562
C	282	GLY	-	cloning artifact	GB 15601562
C	283	GLY	-	cloning artifact	GB 15601562
C	284	SER	-	cloning artifact	GB 15601562
C	285	HIS	-	cloning artifact	GB 15601562
C	286	HIS	-	cloning artifact	GB 15601562
C	287	HIS	-	cloning artifact	GB 15601562
C	288	HIS	-	cloning artifact	GB 15601562

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Chain	Residue	Modelled	Actual	Comment	Reference
C	289	HIS	-	cloning artifact	GB 15601562
C	290	HIS	-	cloning artifact	GB 15601562
D	1	MET	-	cloning artifact	GB 15601562
D	2	SER	-	cloning artifact	GB 15601562
D	3	LEU	-	cloning artifact	GB 15601562
D	42	MSE	MET	modified residue	GB 15601562
D	81	MSE	MET	modified residue	GB 15601562
D	163	MSE	MET	modified residue	GB 15601562
D	189	MSE	MET	modified residue	GB 15601562
D	190	MSE	MET	modified residue	GB 15601562
D	275	MSE	MET	modified residue	GB 15601562
D	281	GLU	-	cloning artifact	GB 15601562
D	282	GLY	-	cloning artifact	GB 15601562
D	283	GLY	-	cloning artifact	GB 15601562
D	284	SER	-	cloning artifact	GB 15601562
D	285	HIS	-	cloning artifact	GB 15601562
D	286	HIS	-	cloning artifact	GB 15601562
D	287	HIS	-	cloning artifact	GB 15601562
D	288	HIS	-	cloning artifact	GB 15601562
D	289	HIS	-	cloning artifact	GB 15601562
D	290	HIS	-	cloning artifact	GB 15601562
E	1	MET	-	cloning artifact	GB 15601562
E	2	SER	-	cloning artifact	GB 15601562
E	3	LEU	-	cloning artifact	GB 15601562
E	42	MSE	MET	modified residue	GB 15601562
E	81	MSE	MET	modified residue	GB 15601562
E	163	MSE	MET	modified residue	GB 15601562
E	189	MSE	MET	modified residue	GB 15601562
E	190	MSE	MET	modified residue	GB 15601562
E	275	MSE	MET	modified residue	GB 15601562
E	281	GLU	-	cloning artifact	GB 15601562
E	282	GLY	-	cloning artifact	GB 15601562
E	283	GLY	-	cloning artifact	GB 15601562
E	284	SER	-	cloning artifact	GB 15601562
E	285	HIS	-	cloning artifact	GB 15601562
E	286	HIS	-	cloning artifact	GB 15601562
E	287	HIS	-	cloning artifact	GB 15601562
E	288	HIS	-	cloning artifact	GB 15601562
E	289	HIS	-	cloning artifact	GB 15601562
E	290	HIS	-	cloning artifact	GB 15601562
F	1	MET	-	cloning artifact	GB 15601562
F	2	SER	-	cloning artifact	GB 15601562

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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	LEU	-	cloning artifact	GB 15601562
F	42	MSE	MET	modified residue	GB 15601562
F	81	MSE	MET	modified residue	GB 15601562
F	163	MSE	MET	modified residue	GB 15601562
F	189	MSE	MET	modified residue	GB 15601562
F	190	MSE	MET	modified residue	GB 15601562
F	275	MSE	MET	modified residue	GB 15601562
F	281	GLU	-	cloning artifact	GB 15601562
F	282	GLY	-	cloning artifact	GB 15601562
F	283	GLY	-	cloning artifact	GB 15601562
F	284	SER	-	cloning artifact	GB 15601562
F	285	HIS	-	cloning artifact	GB 15601562
F	286	HIS	-	cloning artifact	GB 15601562
F	287	HIS	-	cloning artifact	GB 15601562
F	288	HIS	-	cloning artifact	GB 15601562
F	289	HIS	-	cloning artifact	GB 15601562
F	290	HIS	-	cloning artifact	GB 15601562
G	1	MET	-	cloning artifact	GB 15601562
G	2	SER	-	cloning artifact	GB 15601562
G	3	LEU	-	cloning artifact	GB 15601562
G	42	MSE	MET	modified residue	GB 15601562
G	81	MSE	MET	modified residue	GB 15601562
G	163	MSE	MET	modified residue	GB 15601562
G	189	MSE	MET	modified residue	GB 15601562
G	190	MSE	MET	modified residue	GB 15601562
G	275	MSE	MET	modified residue	GB 15601562
G	281	GLU	-	cloning artifact	GB 15601562
G	282	GLY	-	cloning artifact	GB 15601562
G	283	GLY	-	cloning artifact	GB 15601562
G	284	SER	-	cloning artifact	GB 15601562
G	285	HIS	-	cloning artifact	GB 15601562
G	286	HIS	-	cloning artifact	GB 15601562
G	287	HIS	-	cloning artifact	GB 15601562
G	288	HIS	-	cloning artifact	GB 15601562
G	289	HIS	-	cloning artifact	GB 15601562
G	290	HIS	-	cloning artifact	GB 15601562
H	1	MET	-	cloning artifact	GB 15601562
H	2	SER	-	cloning artifact	GB 15601562
H	3	LEU	-	cloning artifact	GB 15601562
H	42	MSE	MET	modified residue	GB 15601562
H	81	MSE	MET	modified residue	GB 15601562
H	163	MSE	MET	modified residue	GB 15601562

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Chain	Residue	Modelled	Actual	Comment	Reference
H	189	MSE	MET	modified residue	GB 15601562
H	190	MSE	MET	modified residue	GB 15601562
H	275	MSE	MET	modified residue	GB 15601562
H	281	GLU	-	cloning artifact	GB 15601562
H	282	GLY	-	cloning artifact	GB 15601562
H	283	GLY	-	cloning artifact	GB 15601562
H	284	SER	-	cloning artifact	GB 15601562
H	285	HIS	-	cloning artifact	GB 15601562
H	286	HIS	-	cloning artifact	GB 15601562
H	287	HIS	-	cloning artifact	GB 15601562
H	288	HIS	-	cloning artifact	GB 15601562
H	289	HIS	-	cloning artifact	GB 15601562
H	290	HIS	-	cloning artifact	GB 15601562

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
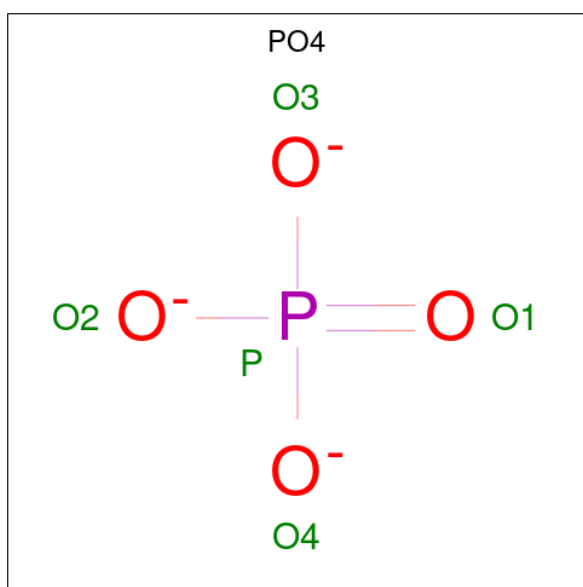
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 5	O 4	P 1	0	0
2	G	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

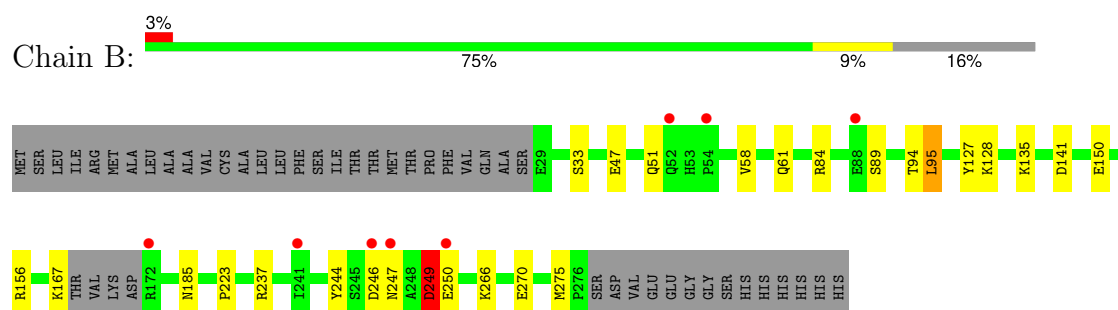| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total 177	O 177	0	0
4	B	190	Total 190	O 190	0	0
4	C	159	Total 159	O 159	0	0
4	D	145	Total 145	O 145	0	0
4	E	160	Total 160	O 160	0	0
4	F	216	Total 216	O 216	0	0
4	G	163	Total 163	O 163	0	0
4	H	202	Total 202	O 202	0	0

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.
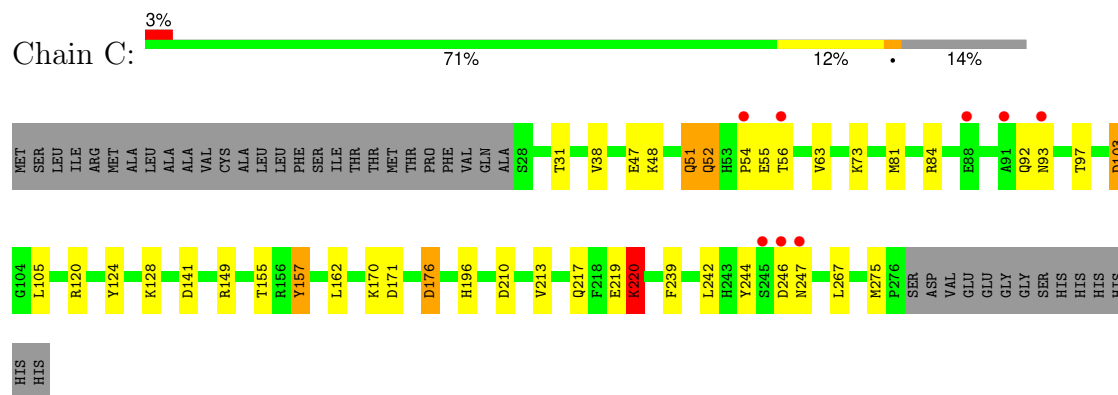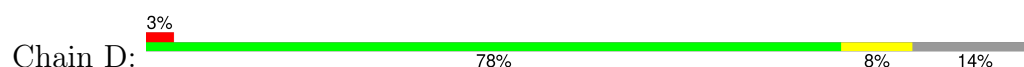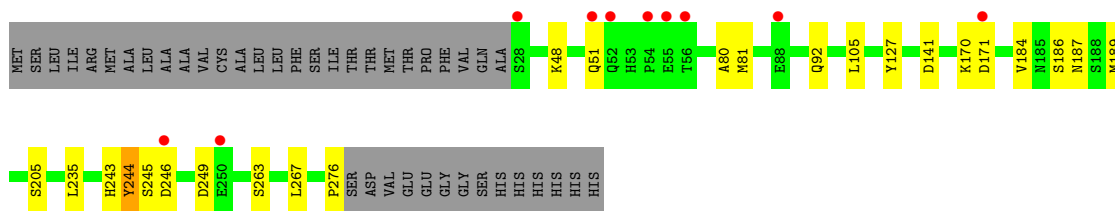
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

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MET SER LEU ILE ARG MET ALA LEU ALA ALA VAL CYS ALA LEU LEU PHE SER ILE THR THR MET THR PRO PHE VAL GLN ALA S28 K48 Q51 Q52 H53 P54 E55 T56 A80 M81 E88 Q92 L105 Y127 D141 K170 D171 V184 N185 S186 N187 S188 M189

S205 L235 H243 Y244 S245 D246 D249 E250 S263 L267 P276 SER ASP VAL GLU GLY GLY SER HIS HIS HIS HIS HIS HIS

- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain E:

MET SER LEU ILE ARG MET ALA LEU ALA ALA VAL CYS ALA LEU LEU PHE SER ILE THR THR MET THR PRO PHE VAL GLN ALA SER E29 K48 T56 V76 A77 D78 E88 S89 N93 H96 Y127 K128 N133 D141 Q142 K143 R149 Y157 E160

K167 D171 R172 D176 L193 Q217 D226 L235 L242 S245 D246 E250 Q251 Y273 P276 SER ASP VAL GLU GLU GLY SER HIS HIS HIS HIS HIS HIS

- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain F:

MET SER LEU ILE ARG MET ALA LEU ALA ALA VAL CYS ALA LEU LEU PHE SER ILE THR THR MET THR PRO PHE VAL GLN ALA S28 S33 E47 K48 Q51 Q52 E55 T56 Y57 Q61 K74 D78 M81 T82 S83 R84 Y85 E88 N93 F98 G104

E121 Y127 D141 S158 F159 E160 T168 VAL LYS D171 R172 E173 V174 S188 I206 F218 E219 Y233 Q234 L235 P238 L242 N247 A248 S263 K266 Y271 M275 P276 SER ASP VAL GLU GLU GLY SER HIS HIS HIS HIS HIS HIS
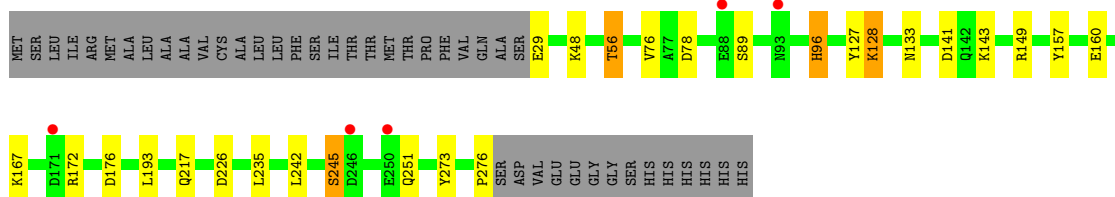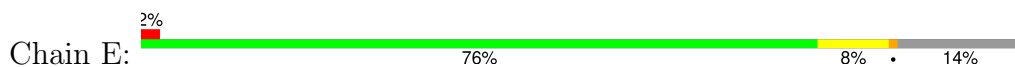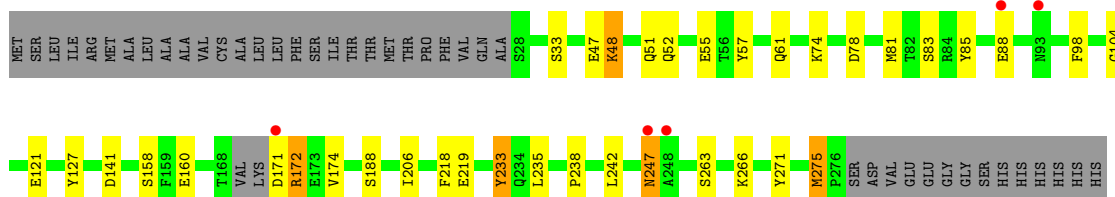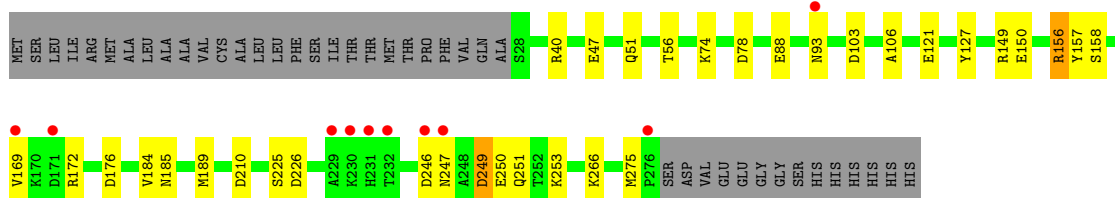
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain G:

MET SER LEU ILE ARG MET ALA LEU ALA ALA VAL CYS ALA LEU LEU PHE SER ILE THR THR MET THR PRO PHE VAL GLN ALA S28 R40 E47 Q51 T56 K74 D78 E88 N93 D103 A106 E121 Y127 R149 E150 R156 Y157 S158

V169 K170 D171 R172 D176 V184 N185 M189 D210 S225 D226 A229 K230 H231 T232 D246 N247 A248 D249 E250 Q251 T252 K253 K266 M275 P276 SER ASP VAL GLU GLU GLY GLY SER HIS HIS HIS HIS HIS

- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain H:

MET SER LEU ILE ARG MET ALA LEU ALA ALA VAL CYS ALA LEU LEU PHE SER ILE THR THR MET THR PRO PHE VAL GLN ALA S28 K48 Q51 E55 T56 L71 V76 A77 D78 E88 N93 H96 Q111 R120 Y127 K135 E150 Y157

K170 D171 R172 E173 V174 N195 H196 I206 D226 R237 H243 Y244 S245 D246 N247 Q251 E254 L259 K266 L267 E270 Y273 I274 M275 P276 SER ASP VAL GLU GLU GLY SER HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.63Å 103.93Å 126.69Å 90.00° 102.35° 90.00°	Depositor
Resolution (Å)	19.73 – 1.65 24.84 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.73-1.65) 99.7 (24.84-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$<I/\sigma(I)>$ [1]	2.77 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.193 , 0.231 0.202 , 0.236	Depositor DCC
R_{free} test set	7739 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16805	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PO4, 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	1.32	6/1947 (0.3%)	1.18	9/2626 (0.3%)
1	B	1.36	3/1922 (0.2%)	1.19	7/2592 (0.3%)
1	C	1.37	6/1982 (0.3%)	1.25	14/2674 (0.5%)
1	D	1.26	5/1942 (0.3%)	1.14	5/2621 (0.2%)
1	E	1.31	4/1949 (0.2%)	1.22	8/2629 (0.3%)
1	F	1.38	15/1947 (0.8%)	1.22	7/2625 (0.3%)
1	G	1.31	7/1956 (0.4%)	1.22	12/2638 (0.5%)
1	H	1.36	3/1984 (0.2%)	1.24	10/2676 (0.4%)
All	All	1.33	49/15629 (0.3%)	1.21	72/21081 (0.3%)

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	C	0	1
1	G	0	1
All	All	0	2

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	121	GLU	CD-OE1	9.52	1.36	1.25
1	G	121	GLU	CD-OE1	9.17	1.35	1.25
1	B	275	MSE	SE-CE	-7.96	1.48	1.95
1	F	174	VAL	CB-CG2	-7.59	1.36	1.52
1	F	55	GLU	CD-OE2	7.32	1.33	1.25

The worst 5 of 72 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	E	276	PRO	CA-C-O	-9.72	96.88	120.20
1	G	156	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	G	156	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	156	ARG	NE-CZ-NH2	-9.46	115.57	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	HIS	Sidechain
1	G	246	ASP	Peptide

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	1919	0	1927	7	0
1	B	1890	0	1891	8	0
1	C	1937	0	1937	23	0
1	D	1918	0	1926	10	0
1	E	1917	0	1924	12	0
1	F	1910	0	1908	14	0
1	G	1924	0	1929	7	0
1	H	1937	0	1950	20	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	1	0	0	0	0
4	A	177	0	0	3	0
4	B	190	0	0	4	0
4	C	159	0	0	7	0
4	D	145	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	160	0	0	1	0
4	F	216	0	0	5	0
4	G	163	0	0	2	0
4	H	202	0	0	7	0
All	All	16805	0	15392	95	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 3.

The worst 5 of 95 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:C:103[B]:ASP:OD1	4:C:1560:HOH:O	1.57	1.15
2:C:1507:PO4:O3	4:C:1666:HOH:O	1.75	1.05
1:H:266[B]:LYS:HD2	4:H:1568:HOH:O	1.55	1.04
1:B:61:GLN:HG3	4:B:1686:HOH:O	1.69	0.91
1:C:31:THR:HG23	4:C:1647:HOH:O	1.75	0.85

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	248/290 (86%)	242 (98%)	6 (2%)	0	100	100
1	B	242/290 (83%)	238 (98%)	3 (1%)	1 (0%)	34	16
1	C	252/290 (87%)	245 (97%)	7 (3%)	0	100	100
1	D	247/290 (85%)	243 (98%)	4 (2%)	0	100	100
1	E	248/290 (86%)	239 (96%)	8 (3%)	1 (0%)	34	16
1	F	246/290 (85%)	241 (98%)	4 (2%)	1 (0%)	34	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	249/290 (86%)	243 (98%)	6 (2%)	0	100	100
1	H	252/290 (87%)	249 (99%)	3 (1%)	0	100	100
All	All	1984/2320 (86%)	1940 (98%)	41 (2%)	3 (0%)	47	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	245	SER
1	F	172	ARG
1	B	249	ASP

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	214/241 (89%)	205 (96%)	9 (4%)	30	8
1	B	210/241 (87%)	197 (94%)	13 (6%)	18	3
1	C	218/241 (90%)	212 (97%)	6 (3%)	43	18
1	D	213/241 (88%)	208 (98%)	5 (2%)	50	25
1	E	214/241 (89%)	208 (97%)	6 (3%)	43	18
1	F	214/241 (89%)	206 (96%)	8 (4%)	34	10
1	G	215/241 (89%)	205 (95%)	10 (5%)	26	6
1	H	218/241 (90%)	208 (95%)	10 (5%)	27	6
All	All	1716/1928 (89%)	1649 (96%)	67 (4%)	33	9

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	28	SER
1	H	88	GLU
1	H	206	ILE
1	C	52	GLN

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Mol	Chain	Res	Type
1	C	51	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	251	GLN
1	H	93	ASN
1	D	61	GLN
1	C	251	GLN
1	H	96	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is 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	#$|Z| > 2$
2	PO4	G	1505	-	4,4,4	1.53	1 (25%)	6,6,6	1.03	0
2	PO4	B	1501	-	4,4,4	1.36	1 (25%)	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	PO4	A	1500	-	4,4,4	1.87	1 (25%)	6,6,6	0.96	0
2	PO4	H	1506	-	4,4,4	1.40	1 (25%)	6,6,6	1.21	1 (16%)
2	PO4	C	1507	-	4,4,4	0.63	0	6,6,6	1.06	0
2	PO4	D	1502	-	4,4,4	0.80	0	6,6,6	0.99	0
2	PO4	E	1503	-	4,4,4	1.88	1 (25%)	6,6,6	1.21	1 (16%)
2	PO4	F	1504	-	4,4,4	1.16	0	6,6,6	1.36	1 (16%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1503	PO4	P-O2	3.33	1.64	1.54
2	A	1500	PO4	P-O2	3.07	1.63	1.54
2	B	1501	PO4	P-O1	2.53	1.56	1.50
2	G	1505	PO4	P-O2	-2.36	1.47	1.54
2	H	1506	PO4	P-O2	2.03	1.60	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1504	PO4	O3-P-O2	2.81	116.65	107.91
2	H	1506	PO4	O2-P-O1	-2.06	103.68	110.95
2	E	1503	PO4	O3-P-O1	-2.03	103.77	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1507	PO4	2	0

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	243/290 (83%)	-0.05	9 (3%)	41	41	14, 22, 49, 63	0
1	B	238/290 (82%)	0.07	8 (3%)	45	45	14, 23, 50, 71	0
1	C	243/290 (83%)	0.12	8 (3%)	46	47	13, 26, 52, 82	0
1	D	243/290 (83%)	0.06	10 (4%)	37	37	15, 27, 54, 71	0
1	E	242/290 (83%)	-0.03	5 (2%)	63	65	15, 26, 46, 55	0
1	F	241/290 (83%)	-0.16	5 (2%)	63	65	13, 20, 43, 62	0
1	G	243/290 (83%)	0.05	10 (4%)	37	37	13, 24, 51, 67	0
1	H	243/290 (83%)	-0.14	5 (2%)	63	65	15, 22, 39, 54	0
All	All	1936/2320 (83%)	-0.01	60 (3%)	49	49	13, 24, 49, 82	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	6.1
1	C	247	ASN	5.9
1	C	93	ASN	5.4
1	G	229	ALA	4.7
1	A	246	ASP	4.5

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, 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
2	PO4	C	1507	5/5	0.89	0.15	19,24,32,33	5
3	MG	A	1508	1/1	0.97	0.08	32,32,32,32	0
2	PO4	D	1502	5/5	0.98	0.06	20,21,23,24	0
2	PO4	E	1503	5/5	0.98	0.06	21,22,24,24	0
2	PO4	A	1500	5/5	0.98	0.06	18,19,21,24	0
2	PO4	F	1504	5/5	0.99	0.04	17,20,20,22	0
2	PO4	G	1505	5/5	0.99	0.06	17,18,19,22	0
2	PO4	H	1506	5/5	0.99	0.05	17,17,21,21	0
2	PO4	B	1501	5/5	0.99	0.06	18,18,19,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.