wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2024 – 02:15 PM EDT

PDB ID	:	3ZSF
Title	:	Crystal structure of the L-cystine solute receptor of Neisseria gonorrhoeae in the unliganded open conformation
Authors	:	Bulut, H.; Moniot, S.; Scheffel, F.; Gathmann, S.; Licht, A.; Saenger, W.; Schneider, E.
Deposited on	:	2011-06-27
Resolution	:	2.32 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 (1)) were used in the production of this report:

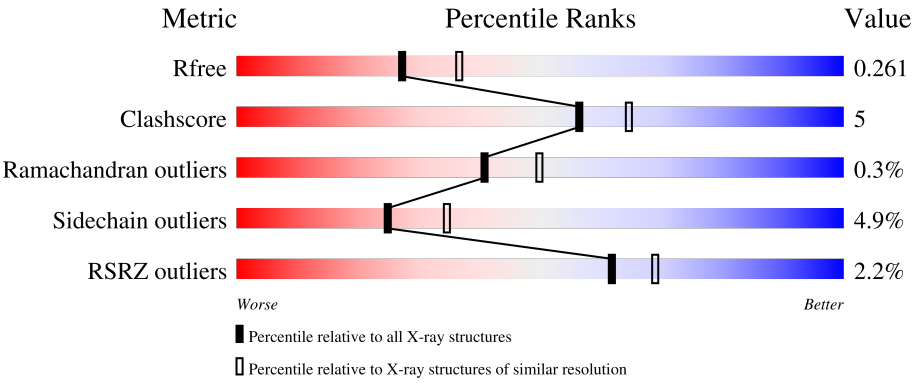
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	283	77% 6% 16%
1	B	283	5% 72% 9% 16%
1	C	283	72% 11% 17%
1	D	283	% 73% 9% 16%
1	E	283	72% 12% 16%

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Mol	Chain	Length	Quality of chain
1	F	283	2% 73% 10% 16%
1	G	283	72% 11% 17%
1	H	283	6% 74% 8% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14685 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 BINDING PROTEIN, AMINO ACID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	2	0
			1793	1128	302	361	2			
1	B	237	Total	C	N	O	S	0	1	0
			1756	1102	295	357	2			
1	C	235	Total	C	N	O	S	0	0	0
			1756	1106	297	351	2			
1	D	237	Total	C	N	O	S	0	0	0
			1763	1108	300	353	2			
1	E	237	Total	C	N	O	S	0	1	0
			1786	1124	302	357	3			
1	F	238	Total	C	N	O	S	0	1	0
			1757	1103	299	353	2			
1	G	235	Total	C	N	O	S	0	3	0
			1771	1115	299	355	2			
1	H	236	Total	C	N	O	S	0	0	0
			1724	1084	291	347	2			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q5F9M1
A	-6	GLY	-	expression tag	UNP Q5F9M1
A	-5	HIS	-	expression tag	UNP Q5F9M1
A	-4	HIS	-	expression tag	UNP Q5F9M1
A	-3	HIS	-	expression tag	UNP Q5F9M1
A	-2	HIS	-	expression tag	UNP Q5F9M1
A	-1	HIS	-	expression tag	UNP Q5F9M1
A	0	HIS	-	expression tag	UNP Q5F9M1
A	1	HIS	-	expression tag	UNP Q5F9M1
A	2	HIS	-	expression tag	UNP Q5F9M1
A	3	HIS	-	expression tag	UNP Q5F9M1
A	4	HIS	-	expression tag	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	expression tag	UNP Q5F9M1
A	6	SER	-	expression tag	UNP Q5F9M1
A	7	GLY	-	expression tag	UNP Q5F9M1
A	8	HIS	-	expression tag	UNP Q5F9M1
A	9	ILE	-	expression tag	UNP Q5F9M1
A	10	ASP	-	expression tag	UNP Q5F9M1
A	11	ASP	-	expression tag	UNP Q5F9M1
A	12	ASP	-	expression tag	UNP Q5F9M1
A	13	ASP	-	expression tag	UNP Q5F9M1
A	14	LYS	-	expression tag	UNP Q5F9M1
A	15	HIS	-	expression tag	UNP Q5F9M1
A	16	MET	-	expression tag	UNP Q5F9M1
A	19	ALA	CYS	engineered mutation	UNP Q5F9M1
B	-7	MET	-	expression tag	UNP Q5F9M1
B	-6	GLY	-	expression tag	UNP Q5F9M1
B	-5	HIS	-	expression tag	UNP Q5F9M1
B	-4	HIS	-	expression tag	UNP Q5F9M1
B	-3	HIS	-	expression tag	UNP Q5F9M1
B	-2	HIS	-	expression tag	UNP Q5F9M1
B	-1	HIS	-	expression tag	UNP Q5F9M1
B	0	HIS	-	expression tag	UNP Q5F9M1
B	1	HIS	-	expression tag	UNP Q5F9M1
B	2	HIS	-	expression tag	UNP Q5F9M1
B	3	HIS	-	expression tag	UNP Q5F9M1
B	4	HIS	-	expression tag	UNP Q5F9M1
B	5	SER	-	expression tag	UNP Q5F9M1
B	6	SER	-	expression tag	UNP Q5F9M1
B	7	GLY	-	expression tag	UNP Q5F9M1
B	8	HIS	-	expression tag	UNP Q5F9M1
B	9	ILE	-	expression tag	UNP Q5F9M1
B	10	ASP	-	expression tag	UNP Q5F9M1
B	11	ASP	-	expression tag	UNP Q5F9M1
B	12	ASP	-	expression tag	UNP Q5F9M1
B	13	ASP	-	expression tag	UNP Q5F9M1
B	14	LYS	-	expression tag	UNP Q5F9M1
B	15	HIS	-	expression tag	UNP Q5F9M1
B	16	MET	-	expression tag	UNP Q5F9M1
B	19	ALA	CYS	engineered mutation	UNP Q5F9M1
C	-7	MET	-	expression tag	UNP Q5F9M1
C	-6	GLY	-	expression tag	UNP Q5F9M1
C	-5	HIS	-	expression tag	UNP Q5F9M1
C	-4	HIS	-	expression tag	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP Q5F9M1
C	-2	HIS	-	expression tag	UNP Q5F9M1
C	-1	HIS	-	expression tag	UNP Q5F9M1
C	0	HIS	-	expression tag	UNP Q5F9M1
C	1	HIS	-	expression tag	UNP Q5F9M1
C	2	HIS	-	expression tag	UNP Q5F9M1
C	3	HIS	-	expression tag	UNP Q5F9M1
C	4	HIS	-	expression tag	UNP Q5F9M1
C	5	SER	-	expression tag	UNP Q5F9M1
C	6	SER	-	expression tag	UNP Q5F9M1
C	7	GLY	-	expression tag	UNP Q5F9M1
C	8	HIS	-	expression tag	UNP Q5F9M1
C	9	ILE	-	expression tag	UNP Q5F9M1
C	10	ASP	-	expression tag	UNP Q5F9M1
C	11	ASP	-	expression tag	UNP Q5F9M1
C	12	ASP	-	expression tag	UNP Q5F9M1
C	13	ASP	-	expression tag	UNP Q5F9M1
C	14	LYS	-	expression tag	UNP Q5F9M1
C	15	HIS	-	expression tag	UNP Q5F9M1
C	16	MET	-	expression tag	UNP Q5F9M1
C	19	ALA	CYS	engineered mutation	UNP Q5F9M1
D	-7	MET	-	expression tag	UNP Q5F9M1
D	-6	GLY	-	expression tag	UNP Q5F9M1
D	-5	HIS	-	expression tag	UNP Q5F9M1
D	-4	HIS	-	expression tag	UNP Q5F9M1
D	-3	HIS	-	expression tag	UNP Q5F9M1
D	-2	HIS	-	expression tag	UNP Q5F9M1
D	-1	HIS	-	expression tag	UNP Q5F9M1
D	0	HIS	-	expression tag	UNP Q5F9M1
D	1	HIS	-	expression tag	UNP Q5F9M1
D	2	HIS	-	expression tag	UNP Q5F9M1
D	3	HIS	-	expression tag	UNP Q5F9M1
D	4	HIS	-	expression tag	UNP Q5F9M1
D	5	SER	-	expression tag	UNP Q5F9M1
D	6	SER	-	expression tag	UNP Q5F9M1
D	7	GLY	-	expression tag	UNP Q5F9M1
D	8	HIS	-	expression tag	UNP Q5F9M1
D	9	ILE	-	expression tag	UNP Q5F9M1
D	10	ASP	-	expression tag	UNP Q5F9M1
D	11	ASP	-	expression tag	UNP Q5F9M1
D	12	ASP	-	expression tag	UNP Q5F9M1
D	13	ASP	-	expression tag	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	14	LYS	-	expression tag	UNP Q5F9M1
D	15	HIS	-	expression tag	UNP Q5F9M1
D	16	MET	-	expression tag	UNP Q5F9M1
D	19	ALA	CYS	engineered mutation	UNP Q5F9M1
E	-7	MET	-	expression tag	UNP Q5F9M1
E	-6	GLY	-	expression tag	UNP Q5F9M1
E	-5	HIS	-	expression tag	UNP Q5F9M1
E	-4	HIS	-	expression tag	UNP Q5F9M1
E	-3	HIS	-	expression tag	UNP Q5F9M1
E	-2	HIS	-	expression tag	UNP Q5F9M1
E	-1	HIS	-	expression tag	UNP Q5F9M1
E	0	HIS	-	expression tag	UNP Q5F9M1
E	1	HIS	-	expression tag	UNP Q5F9M1
E	2	HIS	-	expression tag	UNP Q5F9M1
E	3	HIS	-	expression tag	UNP Q5F9M1
E	4	HIS	-	expression tag	UNP Q5F9M1
E	5	SER	-	expression tag	UNP Q5F9M1
E	6	SER	-	expression tag	UNP Q5F9M1
E	7	GLY	-	expression tag	UNP Q5F9M1
E	8	HIS	-	expression tag	UNP Q5F9M1
E	9	ILE	-	expression tag	UNP Q5F9M1
E	10	ASP	-	expression tag	UNP Q5F9M1
E	11	ASP	-	expression tag	UNP Q5F9M1
E	12	ASP	-	expression tag	UNP Q5F9M1
E	13	ASP	-	expression tag	UNP Q5F9M1
E	14	LYS	-	expression tag	UNP Q5F9M1
E	15	HIS	-	expression tag	UNP Q5F9M1
E	16	MET	-	expression tag	UNP Q5F9M1
E	19	ALA	CYS	engineered mutation	UNP Q5F9M1
F	-7	MET	-	expression tag	UNP Q5F9M1
F	-6	GLY	-	expression tag	UNP Q5F9M1
F	-5	HIS	-	expression tag	UNP Q5F9M1
F	-4	HIS	-	expression tag	UNP Q5F9M1
F	-3	HIS	-	expression tag	UNP Q5F9M1
F	-2	HIS	-	expression tag	UNP Q5F9M1
F	-1	HIS	-	expression tag	UNP Q5F9M1
F	0	HIS	-	expression tag	UNP Q5F9M1
F	1	HIS	-	expression tag	UNP Q5F9M1
F	2	HIS	-	expression tag	UNP Q5F9M1
F	3	HIS	-	expression tag	UNP Q5F9M1
F	4	HIS	-	expression tag	UNP Q5F9M1
F	5	SER	-	expression tag	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	6	SER	-	expression tag	UNP Q5F9M1
F	7	GLY	-	expression tag	UNP Q5F9M1
F	8	HIS	-	expression tag	UNP Q5F9M1
F	9	ILE	-	expression tag	UNP Q5F9M1
F	10	ASP	-	expression tag	UNP Q5F9M1
F	11	ASP	-	expression tag	UNP Q5F9M1
F	12	ASP	-	expression tag	UNP Q5F9M1
F	13	ASP	-	expression tag	UNP Q5F9M1
F	14	LYS	-	expression tag	UNP Q5F9M1
F	15	HIS	-	expression tag	UNP Q5F9M1
F	16	MET	-	expression tag	UNP Q5F9M1
F	19	ALA	CYS	engineered mutation	UNP Q5F9M1
G	-7	MET	-	expression tag	UNP Q5F9M1
G	-6	GLY	-	expression tag	UNP Q5F9M1
G	-5	HIS	-	expression tag	UNP Q5F9M1
G	-4	HIS	-	expression tag	UNP Q5F9M1
G	-3	HIS	-	expression tag	UNP Q5F9M1
G	-2	HIS	-	expression tag	UNP Q5F9M1
G	-1	HIS	-	expression tag	UNP Q5F9M1
G	0	HIS	-	expression tag	UNP Q5F9M1
G	1	HIS	-	expression tag	UNP Q5F9M1
G	2	HIS	-	expression tag	UNP Q5F9M1
G	3	HIS	-	expression tag	UNP Q5F9M1
G	4	HIS	-	expression tag	UNP Q5F9M1
G	5	SER	-	expression tag	UNP Q5F9M1
G	6	SER	-	expression tag	UNP Q5F9M1
G	7	GLY	-	expression tag	UNP Q5F9M1
G	8	HIS	-	expression tag	UNP Q5F9M1
G	9	ILE	-	expression tag	UNP Q5F9M1
G	10	ASP	-	expression tag	UNP Q5F9M1
G	11	ASP	-	expression tag	UNP Q5F9M1
G	12	ASP	-	expression tag	UNP Q5F9M1
G	13	ASP	-	expression tag	UNP Q5F9M1
G	14	LYS	-	expression tag	UNP Q5F9M1
G	15	HIS	-	expression tag	UNP Q5F9M1
G	16	MET	-	expression tag	UNP Q5F9M1
G	19	ALA	CYS	engineered mutation	UNP Q5F9M1
H	-7	MET	-	expression tag	UNP Q5F9M1
H	-6	GLY	-	expression tag	UNP Q5F9M1
H	-5	HIS	-	expression tag	UNP Q5F9M1
H	-4	HIS	-	expression tag	UNP Q5F9M1
H	-3	HIS	-	expression tag	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	HIS	-	expression tag	UNP Q5F9M1
H	-1	HIS	-	expression tag	UNP Q5F9M1
H	0	HIS	-	expression tag	UNP Q5F9M1
H	1	HIS	-	expression tag	UNP Q5F9M1
H	2	HIS	-	expression tag	UNP Q5F9M1
H	3	HIS	-	expression tag	UNP Q5F9M1
H	4	HIS	-	expression tag	UNP Q5F9M1
H	5	SER	-	expression tag	UNP Q5F9M1
H	6	SER	-	expression tag	UNP Q5F9M1
H	7	GLY	-	expression tag	UNP Q5F9M1
H	8	HIS	-	expression tag	UNP Q5F9M1
H	9	ILE	-	expression tag	UNP Q5F9M1
H	10	ASP	-	expression tag	UNP Q5F9M1
H	11	ASP	-	expression tag	UNP Q5F9M1
H	12	ASP	-	expression tag	UNP Q5F9M1
H	13	ASP	-	expression tag	UNP Q5F9M1
H	14	LYS	-	expression tag	UNP Q5F9M1
H	15	HIS	-	expression tag	UNP Q5F9M1
H	16	MET	-	expression tag	UNP Q5F9M1
H	19	ALA	CYS	engineered mutation	UNP Q5F9M1

- Molecule 2 is water.

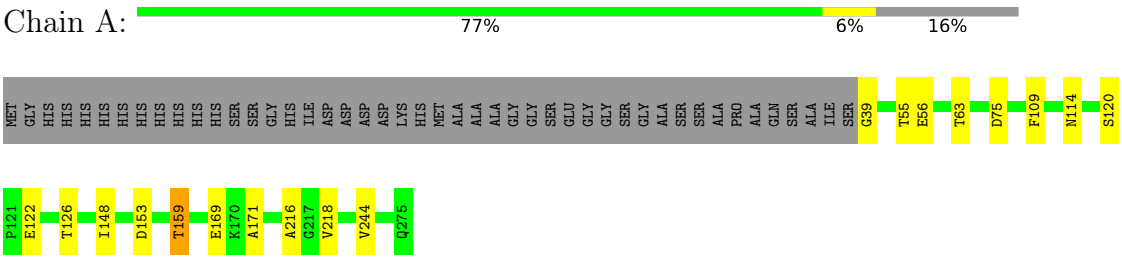
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	83	Total O 83 83	0	0
2	B	60	Total O 60 60	0	0
2	C	74	Total O 74 74	0	0
2	D	63	Total O 63 63	0	0
2	E	85	Total O 85 85	0	0
2	F	64	Total O 64 64	0	0
2	G	83	Total O 83 83	0	0
2	H	67	Total O 67 67	0	0

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.

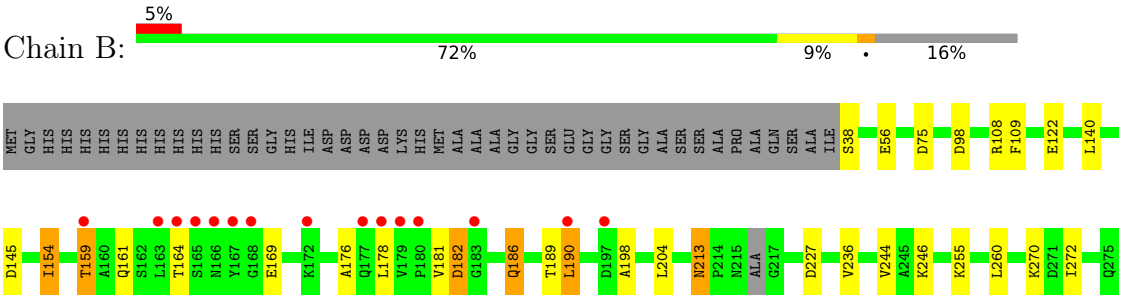
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain A:



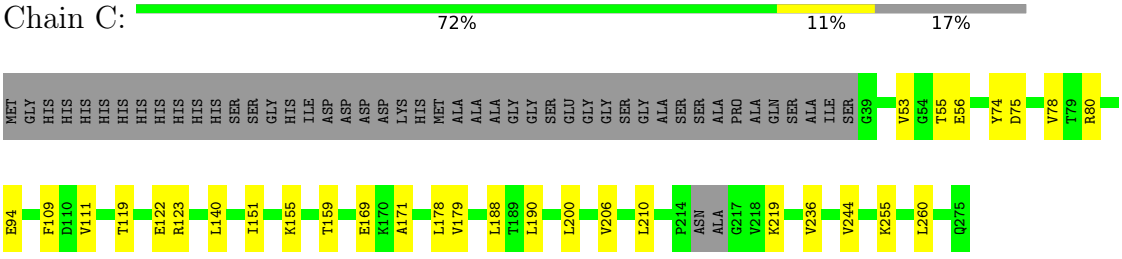
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain B:



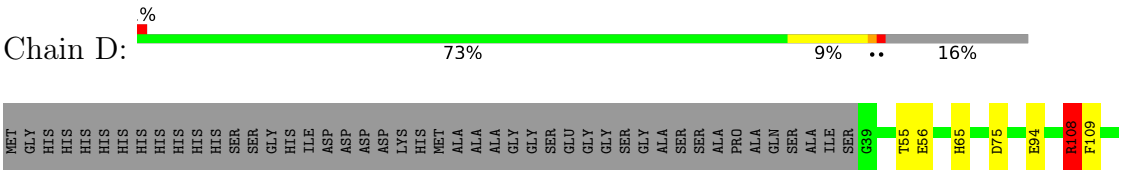
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

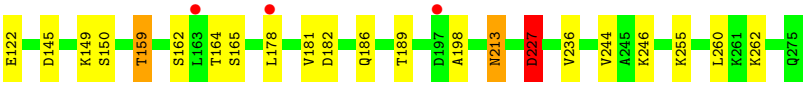
Chain C:



• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

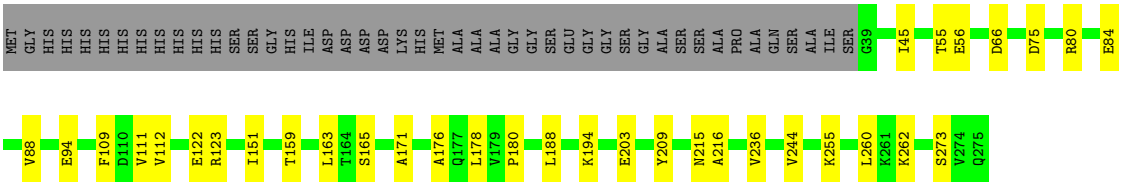
Chain D:





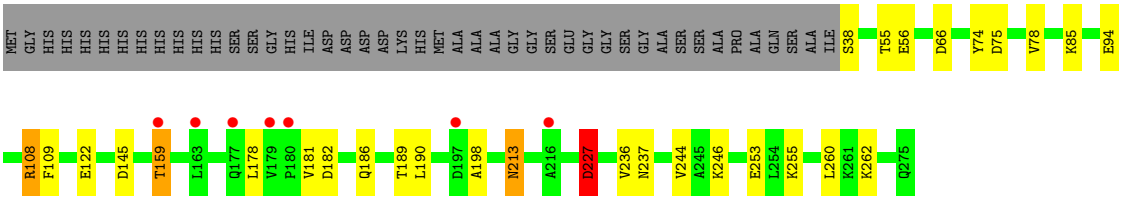
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain E:



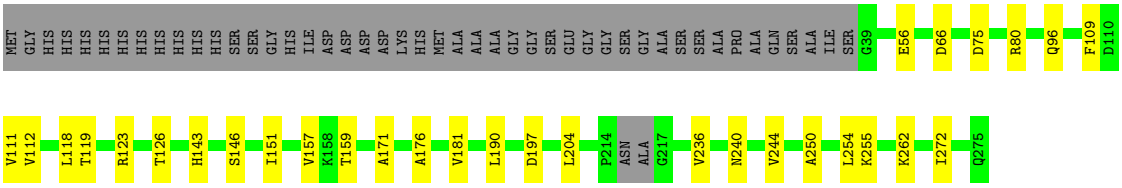
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain F:



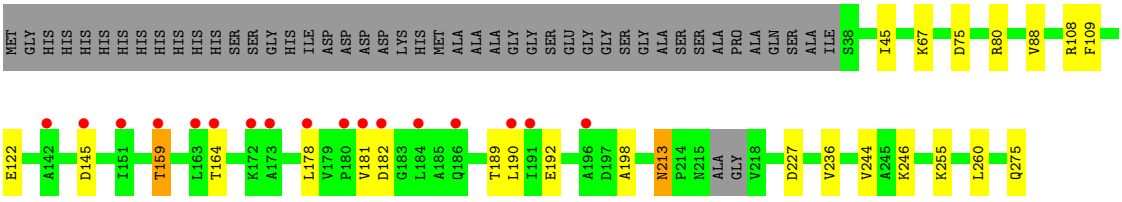
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain G:



• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.09Å 99.83Å 128.83Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	48.00 – 2.32 47.98 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.32) 99.7 (47.98-2.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.267 0.215 , 0.261	Depositor DCC
R_{free} test set	4052 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 13.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14685	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.95	0/1819	0.81	0/2460
1	B	0.86	0/1781	0.94	4/2413 (0.2%)
1	C	0.91	0/1781	0.83	2/2408 (0.1%)
1	D	0.81	0/1789	0.96	5/2421 (0.2%)
1	E	0.97	1/1812 (0.1%)	0.83	1/2449 (0.0%)
1	F	0.80	0/1783	1.01	6/2419 (0.2%)
1	G	0.87	0/1796	0.82	1/2430 (0.0%)
1	H	0.78	0/1749	0.91	4/2371 (0.2%)
All	All	0.87	1/14310 (0.0%)	0.89	23/19371 (0.1%)

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	D	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	203	GLU	CG-CD	5.14	1.59	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	108	ARG	NE-CZ-NH2	-25.72	107.44	120.30
1	D	108	ARG	NE-CZ-NH1	-23.20	108.70	120.30
1	B	108	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	H	108	ARG	NE-CZ-NH2	-18.85	110.87	120.30
1	B	108	ARG	NE-CZ-NH1	16.78	128.69	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	108	ARG	Sidechain
1	F	108	ARG	Sidechain

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	1793	0	1772	12	0
1	B	1756	0	1707	27	0
1	C	1756	0	1743	22	0
1	D	1763	0	1745	17	0
1	E	1786	0	1780	19	0
1	F	1757	0	1714	17	0
1	G	1771	0	1739	23	0
1	H	1724	0	1667	17	0
2	A	83	0	0	3	0
2	B	60	0	0	2	0
2	C	74	0	0	1	0
2	D	63	0	0	1	0
2	E	85	0	0	1	0
2	F	64	0	0	3	0
2	G	83	0	0	2	0
2	H	67	0	0	2	0
All	All	14685	0	13867	140	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 5.

The worst 5 of 140 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:53:VAL:HG22	1:C:111:VAL:CG1	2.02	0.88
1:B:140:LEU:HD21	1:B:154:ILE:HD13	1.55	0.86
1:B:182:ASP:OD1	1:B:186:GLN:HG3	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:VAL:HG21	1:D:244:VAL:HG23	1.61	0.82
1:H:236:VAL:HG21	1:H:244:VAL:HG23	1.63	0.81

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	237/283 (84%)	227 (96%)	9 (4%)	1 (0%)	34 41
1	B	234/283 (83%)	229 (98%)	5 (2%)	0	100 100
1	C	231/283 (82%)	223 (96%)	8 (4%)	0	100 100
1	D	235/283 (83%)	229 (97%)	6 (3%)	0	100 100
1	E	236/283 (83%)	225 (95%)	8 (3%)	3 (1%)	12 12
1	F	237/283 (84%)	232 (98%)	5 (2%)	0	100 100
1	G	234/283 (83%)	226 (97%)	7 (3%)	1 (0%)	34 41
1	H	232/283 (82%)	226 (97%)	6 (3%)	0	100 100
All	All	1876/2264 (83%)	1817 (97%)	54 (3%)	5 (0%)	41 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	215	ASN
1	E	216	ALA
1	E	66	ASP
1	G	146	SER
1	A	114	ASN

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	185/221 (84%)	179 (97%)	6 (3%)	39	53
1	B	180/221 (81%)	166 (92%)	14 (8%)	12	15
1	C	182/221 (82%)	177 (97%)	5 (3%)	44	60
1	D	182/221 (82%)	170 (93%)	12 (7%)	16	22
1	E	186/221 (84%)	179 (96%)	7 (4%)	33	46
1	F	179/221 (81%)	167 (93%)	12 (7%)	16	21
1	G	181/221 (82%)	174 (96%)	7 (4%)	32	45
1	H	173/221 (78%)	165 (95%)	8 (5%)	27	37
All	All	1448/1768 (82%)	1377 (95%)	71 (5%)	25	34

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	109	PHE
1	G	126	THR
1	H	159	THR
1	C	219	LYS
1	C	169	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	47	ASN
1	H	144	ASN
1	B	47	ASN
1	D	47	ASN
1	F	47	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)

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, 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	237/283 (83%)	-0.55	0 100 100	12, 25, 43, 56	0
1	B	237/283 (83%)	-0.09	15 (6%) 20 26	14, 25, 155, 190	0
1	C	235/283 (83%)	-0.58	0 100 100	15, 26, 42, 57	1 (0%)
1	D	237/283 (83%)	-0.36	3 (1%) 77 81	15, 26, 67, 75	0
1	E	237/283 (83%)	-0.55	0 100 100	12, 24, 44, 58	0
1	F	238/283 (84%)	-0.23	7 (2%) 51 59	13, 26, 84, 100	0
1	G	235/283 (83%)	-0.50	0 100 100	15, 28, 48, 68	0
1	H	236/283 (83%)	-0.07	17 (7%) 15 20	13, 27, 101, 115	2 (0%)
All	All	1892/2264 (83%)	-0.36	42 (2%) 62 69	12, 26, 86, 190	3 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	LEU	5.5
1	H	178	LEU	4.9
1	H	163	LEU	4.5
1	B	180	PRO	4.5
1	B	159	THR	4.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.