Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 04:57 am GMT

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 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 (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	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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.

There are no overall percentile quality scores available for this entry.

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

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
			Total	O		
2	A	83	83	83	0	0
			Total	O		
2	B	60	60	60	0	0
			Total	O		
2	C	74	74	74	0	0
			Total	O		
2	D	63	63	63	0	0
			Total	O		
2	E	85	85	85	0	0
			Total	O		
2	F	64	64	64	0	0
			Total	O		
2	G	83	83	83	0	0
			Total	O		
2	H	67	67	67	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	100.0 (48.00-2.32)	Depositor
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	Depositor
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.725	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-l	Xtriage
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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.