



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 02:28 pm GMT

PDB ID : 4APS
Title : Crystal structure of a POT family peptide transporter in an inward open conformation.
Authors : Solcan, N.; Kwok, J.; Fowler, P.W.; Cameron, A.D.; Drew, D.; Iwata, S.; Newstead, S.
Deposited on : 2012-04-05
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

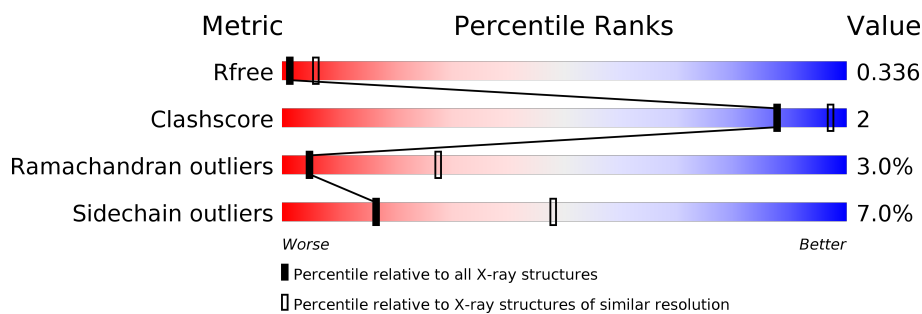
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	491	
1	B	491	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6891 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 DI-OR TRIPEPTIDE H⁺ SYMPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3445	2326	528	574	17			
1	B	446	Total	C	N	O	S	0	0	0
			3445	2326	528	574	17			

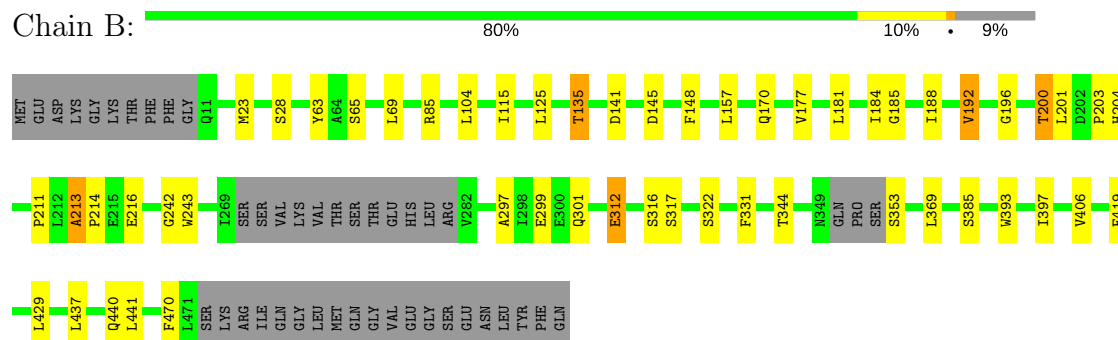
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLY	-	expression tag	UNP Q5M4H8
A	485	SER	-	expression tag	UNP Q5M4H8
A	486	GLU	-	expression tag	UNP Q5M4H8
A	487	ASN	-	expression tag	UNP Q5M4H8
A	488	LEU	-	expression tag	UNP Q5M4H8
A	489	TYR	-	expression tag	UNP Q5M4H8
A	490	PHE	-	expression tag	UNP Q5M4H8
A	491	GLN	-	expression tag	UNP Q5M4H8
B	484	GLY	-	expression tag	UNP Q5M4H8
B	485	SER	-	expression tag	UNP Q5M4H8
B	486	GLU	-	expression tag	UNP Q5M4H8
B	487	ASN	-	expression tag	UNP Q5M4H8
B	488	LEU	-	expression tag	UNP Q5M4H8
B	489	TYR	-	expression tag	UNP Q5M4H8
B	490	PHE	-	expression tag	UNP Q5M4H8
B	491	GLN	-	expression tag	UNP Q5M4H8

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cd	0	0
			1	1		

• Molecule 1: DI-OR TRIPEPTIDE H⁺ SYMPORTER



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.39Å 112.99Å 215.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.62 – 3.30 22.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.5 (22.62-3.30) 83.8 (22.48-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.94 (at 3.30Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.272 , 0.289 0.324 , 0.336	Depositor DCC
R_{free} test set	1421 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 137.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	6891	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD

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	0.52	0/3549	0.61	0/4844
1	B	0.51	0/3549	0.60	0/4844
All	All	0.52	0/7098	0.61	0/9688

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3445	0	3534	19	0
1	B	3445	0	3534	13	0
2	B	1	0	0	0	0
All	All	6891	0	7068	30	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 2.

All (30) 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:A:165:ILE:HG22	1:A:181:LEU:HD21	1.73	0.70
1:A:331:PHE:HB2	1:A:397:ILE:HD13	1.76	0.67
1:B:331:PHE:HB2	1:B:397:ILE:HD13	1.76	0.66
1:A:135:THR:HG21	1:A:204:HIS:CD2	2.32	0.65
1:A:135:THR:HG21	1:A:204:HIS:HD2	1.62	0.64
1:A:185:GLY:HA2	1:A:188:ILE:HD12	1.81	0.62
1:A:393:TRP:O	1:A:397:ILE:HD12	2.07	0.55
1:B:393:TRP:O	1:B:397:ILE:HD12	2.07	0.54
1:A:20:MET:HB2	1:A:192:VAL:HG11	1.89	0.54
1:A:135:THR:OG1	1:A:204:HIS:NE2	2.37	0.53
1:A:184:ILE:HG23	1:B:184:ILE:HG21	1.93	0.50
1:B:63:TYR:CD1	1:B:115:ILE:HG23	2.48	0.48
1:A:63:TYR:CD1	1:A:115:ILE:HG23	2.49	0.48
1:B:185:GLY:HA2	1:B:188:ILE:HD12	1.96	0.48
1:B:297:ALA:O	1:B:301:GLN:HB2	2.14	0.47
1:A:297:ALA:O	1:A:301:GLN:HB2	2.14	0.47
1:A:20:MET:CB	1:A:192:VAL:HG11	2.46	0.46
1:A:28:SER:OG	1:A:29:TYR:N	2.50	0.45
1:A:213:ALA:HB3	1:A:214:PRO:HD3	1.99	0.44
1:A:25:GLU:OE1	1:A:26:ARG:NE	2.51	0.44
1:B:213:ALA:HB3	1:B:214:PRO:HD3	1.99	0.44
1:B:213:ALA:HB3	1:B:214:PRO:CD	2.49	0.42
1:A:213:ALA:HB3	1:A:214:PRO:CD	2.49	0.42
1:B:135:THR:HG21	1:B:204:HIS:HD2	1.84	0.42
1:A:193:TYR:O	1:A:197:GLY:N	2.50	0.42
1:B:135:THR:HG21	1:B:204:HIS:CD2	2.54	0.42
1:B:192:VAL:O	1:B:196:GLY:N	2.51	0.41
1:B:135:THR:HG1	1:B:204:HIS:CD2	2.39	0.40
1:A:191:LEU:HG	1:B:177:VAL:HG13	2.04	0.40
1:A:31:GLY:CA	1:A:162:ALA:HB1	2.52	0.40

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	440/491 (90%)	406 (92%)	21 (5%)	13 (3%)	5	27
1	B	440/491 (90%)	403 (92%)	24 (6%)	13 (3%)	5	27
All	All	880/982 (90%)	809 (92%)	45 (5%)	26 (3%)	5	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	A	317	SER
1	B	200	THR
1	B	203	PRO
1	B	317	SER
1	A	141	ASP
1	A	200	THR
1	A	385	SER
1	B	141	ASP
1	B	385	SER
1	A	213	ALA
1	A	344	THR
1	A	419	PHE
1	B	213	ALA
1	B	344	THR
1	B	419	PHE
1	A	104	LEU
1	A	312	GLU
1	B	104	LEU
1	B	312	GLU
1	A	125	LEU
1	B	125	LEU
1	A	211	PRO
1	B	211	PRO
1	A	242	GLY
1	B	242	GLY

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	358/398 (90%)	336 (94%)	22 (6%)	20	53
1	B	358/398 (90%)	330 (92%)	28 (8%)	14	42
All	All	716/796 (90%)	666 (93%)	50 (7%)	16	48

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	69	LEU
1	A	135	THR
1	A	145	ASP
1	A	148	PHE
1	A	157	LEU
1	A	200	THR
1	A	201	LEU
1	A	216	GLU
1	A	243	TRP
1	A	299	GLU
1	A	312	GLU
1	A	316	SER
1	A	322	SER
1	A	353	SER
1	A	369	LEU
1	A	406	VAL
1	A	429	LEU
1	A	437	LEU
1	A	440	GLN
1	A	441	LEU
1	A	470	PHE
1	B	23	MET
1	B	28	SER
1	B	65	SER
1	B	69	LEU
1	B	85	ARG
1	B	135	THR
1	B	145	ASP
1	B	148	PHE
1	B	157	LEU
1	B	170	GLN
1	B	181	LEU
1	B	192	VAL
1	B	200	THR

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Mol	Chain	Res	Type
1	B	201	LEU
1	B	216	GLU
1	B	243	TRP
1	B	299	GLU
1	B	312	GLU
1	B	316	SER
1	B	322	SER
1	B	353	SER
1	B	369	LEU
1	B	406	VAL
1	B	429	LEU
1	B	437	LEU
1	B	440	GLN
1	B	441	LEU
1	B	470	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.