Integrative Structure Validation Report

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The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A1E
PDB-Dev ID	PDBDEV_00000086
Structure Title	Integrative structure of the XcpHIJK quaternary complex of a type II secretion system pseudopilin
Structure Authors	Escobar CA; Douzi B; Ball G; Barbat B; Alphonse S; Quinton L; Voulhoux R; Forest KT

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

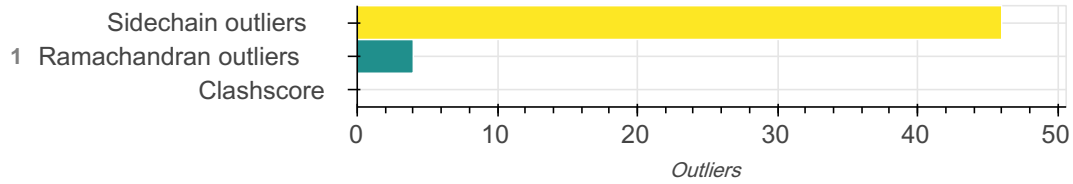
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 4 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 4 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry.This model is titled XcpHIJK model/XcpHIJK.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	XcpH	A	A	131
1	2	2	XcpI	B	B	89
1	3	3	XcpJ	C	C	162
1	4	4	XcpK	D	D	273

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5VTM
2	NMR data	BMRB	50449
3	Crosslinking-MS data	MASSIVE	MSV000086915

ID	Dataset type	Database name	Data access code
4	Comparative model	Not available	Not available
5	Experimental model	PDB	2QV8

Representation

This entry has only one representation and includes 4 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-131	-
B	1-89	-
C	1-162	-
D	1-273	-

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Homology modeling	XcpH modeling	None	None	False	False
2	1	HADDOCK	Docking	None	1000	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Pymol	Not available	Visualization-modeling	https://pymol.org/2/
2	Haddock	Not available	Docking	https://alcazar.science.uu.nl/services/HADDOCK2.2/

ID	Software name	Software version	Software classification	Software location
3	Phyre2	Not available	Homology modeling	http://www.sbg.bio.ic.ac.uk/phyre2/html/page.cgi?id=index

Data quality

NMR

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 881 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
N--HN	0.97	0.86	6
NE2--HE22	0.97	0.86	2
N--HN	0.98	0.86	362
NE2--HE22	0.98	0.86	22
ND2--HD22	0.98	0.86	11
ND2--HD21	0.98	0.86	8
NE2--HE21	0.98	0.86	19
NE2--HE2	0.98	0.86	4
NE--HE	0.98	0.86	30
OH--HH	0.96	0.84	6

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE1--HE1	0.98	0.86	9
OG1--HG1	0.96	0.84	9
OG--HG	0.96	0.84	15
ND1--HD1	0.98	0.86	2
OG--HG	0.97	0.84	9
N--HN	0.99	0.86	63
NE1--HE1	0.99	0.86	5
OG1--HG1	0.97	0.84	3
NE--HE	0.99	0.86	14
OH--HH	0.97	0.84	2
ND2--HD22	0.99	0.86	1
ND2--HD21	0.99	0.86	4
NE2--HE21	0.99	0.86	4
NE2--HE21	1.00	0.86	1
NE2--HE2	1.00	0.86	1
OG--HG	0.98	0.84	3
N--HN	1.00	0.86	1
OG1--HG1	0.98	0.84	2
NE--HE	1.00	0.86	6
NZ--HZ3	1.03	0.89	1
NZ--HZ2	1.03	0.89	1
NZ--HZ2	1.04	0.89	13
NZ--HZ3	1.04	0.89	18

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ1	1.04	0.89	16
NZ--HZ1	1.05	0.89	3
NZ--HZ2	1.05	0.89	5
NH1--HH12	1.03	0.86	1
NH1--HH11	1.03	0.86	1
NH2--HH22	1.03	0.86	1
NH1--HH12	1.04	0.86	34
NH2--HH21	1.04	0.86	26
NH2--HH22	1.04	0.86	30
NH1--HH11	1.04	0.86	28
NH1--HH12	1.05	0.86	13
NH2--HH22	1.05	0.86	13
NH1--HH11	1.05	0.86	13
NH2--HH21	1.05	0.86	15
NH1--HH11	1.06	0.86	8
NH2--HH21	1.06	0.86	9
NH2--HH22	1.06	0.86	6
NH1--HH12	1.06	0.86	1
NH1--HH12	1.07	0.86	1

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	596	568	24	4

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	519	416	57	46

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	B	4	0GLU
1	B	16	0THR
1	B	25	0ASP
1	C	2	0SER
1	C	6	0ASN
1	C	14	0ARG
1	C	26	0SER
1	C	52	0GLN
1	C	60	0GLN
1	C	61	0VAL
1	C	63	0ASP

Model ID	Chain	Residue ID	Residue type
1	C	66	0THR
1	C	69	0SER
1	C	85	0THR
1	C	87	0GLU
1	D	10	0THR
1	D	14	0LEU
1	D	15	0ASP
1	D	36	0LEU
1	D	40	0ARG
1	D	56	0THR
1	D	79	0GLN
1	D	105	0SER
1	D	138	0LEU
1	D	155	0ASP
1	D	168	0ARG
1	D	169	0GLU
1	D	175	0ASP
1	D	178	0THR
1	D	192	0SER
1	D	218	0THR
1	D	228	0ARG
1	D	232	0ARG
1	D	236	0GLN

Model ID	Chain	Residue ID	Residue type
1	A	14	0GLU
1	A	60	0ASP
1	A	68	0SER
1	A	69	0SER
1	A	97	0ARG

Fit of model to data used for modeling

NMR

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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