



Full wwPDB Integrative Structure Validation Report

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

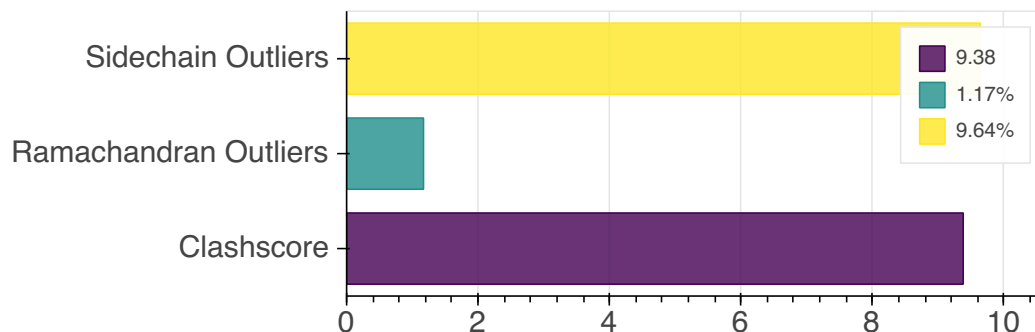
Molprobity : Version 4.4

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000030
Molecule Name	Molecular Architecture of Human Fibrin Clots
Title	Missing regions in the molecular architecture of human fibrin clots structurally resolved by XL-MS and integrative structural modeling
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Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

Summary

This entry consists of 1 unique models, with 13 subunits in each model. A total of 9 datasets or restraints was used to build this entry. Each model is represented by 14 rigid bodies and 7 flexible or non-rigid units.

Entry composition

There is 1 unique type of model in this entry. This model is titled ?/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	RGD-containing Alpha Domain Alpha_558-620	A	63
1	2	2	Subunit Alpha_46-219	B	174
1	3	3	Subunit Alpha_220-249	C	30
1	4	4	Subunit Beta	D	401
1	5	5	Subunit Gamma	E	381
1	6	6	Interactive Alpha Domain Alpha_432-491	F	60
1	7	2	Subunit Alpha_46-219	G	174
1	8	3	Subunit Alpha_220-249	H	30
1	9	7	Beta N-term Beta_55-84	I	34
1	10	4	Subunit Beta	J	401
1	11	5	Subunit Gamma	K	381

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	12	6	Interactive Alpha Domain Alpha_432-491	L	60
1	13	1	RGD-containing Alpha Domain Alpha_558-620	M	63

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	?	?	?	False	False

Data quality

Model quality

Standard geometry

There are 4278 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ3	1.035	0.89	194
NZ--HZ1	1.036	0.89	194
NZ--HZ2	1.035	0.89	194
NH2--HH21	0.997	0.86	103
NH2--HH22	1.001	0.86	103
NH1--HH11	0.999	0.86	103
NH1--HH12	0.998	0.86	103

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OH--HH	0.959	0.84	92
NE--HE	0.981	0.86	103
OG--HG	0.961	0.84	183
ND2--HD21	0.977	0.86	133
OG1--HG1	0.961	0.84	138
NE1--HE1	0.979	0.86	51
NE2--HE2	0.98	0.86	25
NE2--HE21	0.978	0.86	114
N--H	0.974	0.86	2156
ND2--HD22	0.976	0.86	133
NE2--HE22	0.978	0.86	114
ND1--HD1	0.981	0.86	17
SG--HG	1.326	1.2	5

There are 0 angle outliers in this entry.

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
Model 1	9.38	331

All 331 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
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Model ID	Analyzed	Favored	Allowed	Outliers
1	2226	2036	164	26

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:53	PRO
1	B:170	ASN
1	B:190	ASN
1	B:287	ASP
1	B:358	GLY
1	B:437	CYS
1	C:95	ASN
1	C:186	GLY
1	C:365	CYS
1	C:368	GLY
1	C:398	TRP
1	D:53	PRO
1	D:214	PRO
1	D:215	SER
1	E:168	VAL
1	E:172	TYR
1	E:287	ASP
1	E:349	GLY
1	E:379	ALA
1	E:437	CYS

Model ID	Chain and res ID	Residue type
1	F:95	ASN
1	F:186	GLY
1	F:224	LEU
1	F:365	CYS
1	I:613	HIS
1	Z:233	VAL

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	Analysed	Favored	Allowed	Outliers
1	1982	1568	223	191

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	I:559	GLU
1	I:560	SER
1	I:572	SER
1	I:578	SER
1	I:580	SER
1	I:586	SER
1	I:595	THR
1	I:606	GLU
1	I:609	SER
1	I:610	GLU
1	I:618	SER

Model ID	Chain and res ID	Residue type
1	A:55	CYS
1	A:58	GLU
1	A:59	ASP
1	A:63	LYS
1	A:79	GLN
1	A:90	ASN
1	A:92	LEU
1	A:103	HIS
1	A:131	SER
1	A:185	SER
1	A:191	GLU
1	A:203	GLN
1	A:211	ASP
1	Z:223	LEU
1	Z:227	LYS
1	Z:233	VAL
1	Z:239	SER
1	B:108	THR
1	B:118	GLN
1	B:140	THR
1	B:150	LEU
1	B:152	LYS

Model ID	Chain and res ID	Residue type
1	B:159	GLN
1	B:164	ASP
1	B:165	ASN
1	B:170	ASN
1	B:173	SER
1	B:174	SER
1	B:176	LEU
1	B:179	HIS
1	B:186	THR
1	B:193	THR
1	B:211	LYS
1	B:212	LEU
1	B:240	GLU
1	B:243	GLU
1	B:250	GLU
1	B:251	THR
1	B:261	SER
1	B:262	SER
1	B:300	LYS
1	B:310	THR
1	B:332	LEU
1	B:346	ASP
1	B:378	THR

Model ID	Chain and res ID	Residue type
1	B:406	SER
1	B:417	THR
1	B:422	LYS
1	B:423	GLN
1	B:453	THR
1	B:458	LYS
1	B:461	THR
1	B:463	ASP
1	B:473	SER
1	B:484	ILE
1	B:487	PHE
1	C:48	THR
1	C:57	THR
1	C:67	GLN
1	C:99	SER
1	C:119	ILE
1	C:128	THR
1	C:163	GLU
1	C:168	THR
1	C:178	ASP
1	C:209	GLU
1	C:211	ASP
1	C:213	SER

Model ID	Chain and res ID	Residue type
1	C:221	GLN
1	C:224	LEU
1	C:227	SER
1	C:247	THR
1	C:249	THR
1	C:280	ASN
1	C:282	ARG
1	C:296	GLU
1	C:323	ASP
1	C:326	SER
1	C:340	THR
1	C:343	ASN
1	C:349	GLU
1	C:358	SER
1	C:385	THR
1	C:390	ASP
1	C:397	THR
1	C:416	ASN
1	C:419	THR
1	H:432	LYS
1	H:444	THR
1	H:453	SER
1	H:456	THR

Model ID	Chain and res ID	Residue type
1	H:464	THR
1	H:485	SER
1	D:58	GLU
1	D:59	ASP
1	D:63	LYS
1	D:88	LEU
1	D:92	LEU
1	D:93	PHE
1	D:104	SER
1	D:133	ASP
1	D:137	ARG
1	D:155	LEU
1	D:158	ASN
1	D:170	GLU
1	D:185	SER
1	D:190	ARG
1	D:197	TYR
1	D:200	GLN
1	D:203	GLN
1	D:204	LEU
1	Y:231	ASP
1	Y:232	LEU
1	Y:239	SER

Model ID	Chain and res ID	Residue type
1	K:58	SER
1	K:67	SER
1	K:81	THR
1	E:120	GLU
1	E:140	THR
1	E:150	LEU
1	E:159	GLN
1	E:164	ASP
1	E:181	LEU
1	E:199	ARG
1	E:210	GLN
1	E:211	LYS
1	E:225	THR
1	E:240	GLU
1	E:251	THR
1	E:262	SER
1	E:274	THR
1	E:308	THR
1	E:310	THR
1	E:346	ASP
1	E:372	VAL
1	E:396	THR
1	E:406	SER

Model ID	Chain and res ID	Residue type
1	E:418	SER
1	E:461	THR
1	E:463	ASP
1	E:473	SER
1	F:48	THR
1	F:59	GLN
1	F:98	GLU
1	F:99	SER
1	F:128	THR
1	F:175	THR
1	F:211	ASP
1	F:221	GLN
1	F:227	SER
1	F:245	SER
1	F:247	THR
1	F:249	THR
1	F:283	THR
1	F:284	SER
1	F:285	THR
1	F:292	LYS
1	F:303	THR
1	F:326	SER
1	F:339	SER

Model ID	Chain and res ID	Residue type
1	F:354	GLU
1	F:379	THR
1	F:381	SER
1	F:397	THR
1	F:408	THR
1	G:453	SER
1	G:457	THR
1	G:460	SER
1	G:466	THR
1	G:479	THR
1	G:484	THR
1	J:559	GLU
1	J:560	SER
1	J:572	SER
1	J:580	SER
1	J:594	SER
1	J:595	THR
1	J:603	MET
1	J:619	THR
1	J:620	LYS

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model