

Integrative Structure Validation Report ?

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	8ZZU
PDB-Dev ID	PDBDEV_00000030
Structure Title	Molecular Architecture of Human Fibrin Clots
Structure Authors	Oleg Klykov; Carmen van der Zwaan; Albert J.R. Heck; Alexander B. Meijer; Richard A. Scheltema
Deposited on	2019-03-14

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

We welcome your comments at helpdesk@pdb-ihm.org

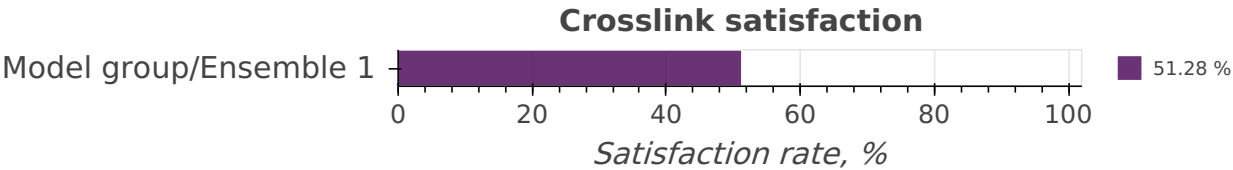
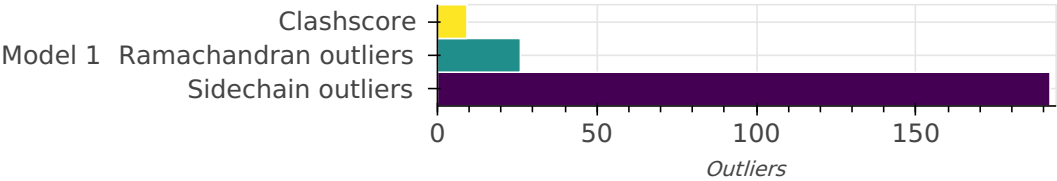
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 and fit to model assessments for SAS and crosslinking-MS 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 model(s). A total of 9 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	RGD-containing Alpha Domain Alpha_558-620	A [I]	63	13-35, 53-63	1-12, 36-52	100.00 / 100.00	Atomic
				M [J]					
		2	Subunit Alpha_46-219	B [A]	174	1-174	-	100.00 / 100.00	Atomic
				G [D]					
		3	Subunit Alpha_220-249	C [Z]	30	1-30	-	100.00 / 100.00	Atomic
				H [Y]					
		4	Subunit Beta	D [B]	401	1-401	-	100.00 / 100.00	Atomic
				J [E]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		5	Subunit Gamma	E [C]	381	1-381	-	100.00 / 100.00	Atomic
				K [F]					
		6	Interactive Alpha Domain Alpha_432-491	F [H]	60	29-60	1-28	100.00 / 100.00	Atomic
				L [G]					
		7	Beta N-term Beta_55-84	I [K]	34	-	1-34	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 9 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	3GHG
2	De Novo model	Not available	Not available
3	De Novo model	Not available	Not available
4	De Novo model	Not available	Not available
5	De Novo model	Not available	Not available
6	Crosslinking-MS data	PRIDE	PXD011680
7	De Novo model	Not available	Not available
8	De Novo model	Not available	Not available
9	De Novo model	Not available	Not available

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	–	–	None	–	False	False

There are 8 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	ThreaDomEx	Not available	None	https://zhanglab.ccmb.med.umich.edu/ThreaDomEx/
2	Robetta	Not available	model building	http://robetta.bakerlab.org
3	HHalign-Kbest	Not available	model building	http://bioserv.rpbs.univ-paris-diderot.fr/services/HHalign-Kbest/
4	I-TASSER	Not available	model building	https://zhanglab.ccmb.med.umich.edu/I-TASSER/
5	RaptorX	Not available	model building	http://raptorx.uchicago.edu
6	HADDOCK	2.20	model building	https://haddock.science.uu.nl
7	CPORT	Not available	None	https://milou.science.uu.nl/services/CPORT/
8	DisVis	Not available	None	https://milou.science.uu.nl/cgi/services/DISVIS/disvis/

Data quality ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

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 no bond length outliers.

Standard geometry: angle outliers ?

There are no bond angle outliers.

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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	9.26	327

There are 327 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:63:LYS:C	I:3:ARG:HD3	1.58	1	1
A:63:LYS:HG3	I:3:ARG:CD	1.52	1	1
A:63:LYS:CG	I:3:ARG:HD2	1.51	1	1
A:60:HIS:CB	I:3:ARG:HH21	1.51	1	1
A:60:HIS:HB3	I:3:ARG:NH2	1.42	1	1
A:61:SER:C	I:3:ARG:HH12	1.31	1	1
A:63:LYS:O	I:3:ARG:HD3	1.24	1	1
A:62:THR:N	I:3:ARG:HH12	1.20	1	1
A:63:LYS:C	I:3:ARG:CD	1.19	1	1
A:63:LYS:CG	I:3:ARG:CD	1.16	1	1
A:60:HIS:C	I:3:ARG:NH2	1.15	1	1
A:63:LYS:O	I:3:ARG:CD	1.15	1	1
A:62:THR:N	I:3:ARG:NH1	1.10	1	1
A:61:SER:C	I:3:ARG:NH1	1.03	1	1
A:12:GLU:HG3	H:18:PHE:CE1	1.03	1	1
A:63:LYS:CB	I:3:ARG:HD2	1.01	1	1
A:61:SER:OG	H:24:LYS:NZ	0.98	1	1
A:63:LYS:HG2	I:3:ARG:HD2	0.97	1	1
C:14:VAL:HG13	C:15:PRO:HD3	0.97	1	1
A:61:SER:N	I:3:ARG:NH2	0.96	1	1
A:63:LYS:CA	I:3:ARG:HD3	0.93	1	1
A:60:HIS:CA	I:3:ARG:NH2	0.93	1	1
A:62:THR:H	I:3:ARG:HH22	0.89	1	1
A:60:HIS:CB	I:3:ARG:NH2	0.89	1	1
A:60:HIS:HB3	I:3:ARG:CZ	0.88	1	1
A:60:HIS:CA	I:3:ARG:HH21	0.87	1	1
A:63:LYS:HG3	I:3:ARG:CG	0.85	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:60:HIS:C	I:3:ARG:CZ	0.84	1	1
A:61:SER:N	I:3:ARG:HH22	0.84	1	1
A:62:THR:H	I:3:ARG:NH2	0.83	1	1
C:25:VAL:HB	C:26:PRO:HD3	0.82	1	1
D:237:LEU:HB3	D:242:ILE:HD11	0.82	1	1
K:238:GLU:HB3	K:368:LYS:HB2	0.82	1	1
A:63:LYS:HE3	I:3:ARG:O	0.80	1	1
A:60:HIS:HB2	I:3:ARG:HE	0.79	1	1
A:63:LYS:CA	I:3:ARG:CD	0.79	1	1
A:63:LYS:HG2	I:3:ARG:CD	0.79	1	1
J:328:TRP:HB2	J:349:ARG:HA	0.75	1	1
E:237:LEU:HB3	E:366:MET:HE2	0.75	1	1
A:22:TYR:C	L:25:THR:HG21	0.74	1	1
D:210:ASP:HB3	D:211:PRO:HD3	0.74	1	1
A:62:THR:N	I:3:ARG:CZ	0.74	1	1
F:10:GLU:HA	F:20:SER:HA	0.74	1	1
J:199:GLN:HA	J:392:LYS:HG2	0.74	1	1
C:12:ASP:HB2	D:70:LYS:HD3	0.73	1	1
A:22:TYR:C	L:25:THR:CG2	0.73	1	1
J:258:GLU:HB3	J:392:LYS:HB2	0.73	1	1
D:311:THR:HB	D:352:ALA:HB2	0.72	1	1
J:125:LEU:HD23	K:111:LEU:HD13	0.70	1	1
A:62:THR:N	I:3:ARG:HH22	0.70	1	1
A:22:TYR:N	L:25:THR:HG21	0.70	1	1
A:60:HIS:CB	I:3:ARG:CZ	0.69	1	1
J:341:ASP:HA	J:376:ASP:HB2	0.69	1	1
D:94:LEU:HD13	J:102:SER:HB3	0.69	1	1
A:63:LYS:CB	I:3:ARG:CD	0.68	1	1
J:246:THR:HB	J:273:THR:HA	0.68	1	1
A:62:THR:N	I:3:ARG:NH2	0.68	1	1
E:374:ILE:HG12	E:375:PRO:HD2	0.68	1	1
K:105:ASN:HA	K:108:ILE:HD12	0.68	1	1
D:90:GLU:O	D:94:LEU:HG	0.67	1	1
A:60:HIS:NE2	H:17:ASN:HA	0.67	1	1
I:21:TYR:HB3	I:24:ARG:HB2	0.66	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:60:HIS:CE1	H:17:ASN:HA	0.66	1	1
D:198:ARG:HB3	D:393:MET:HB3	0.66	1	1
A:48:ASP:HA	A:54:ALA:HB2	0.66	1	1
E:243:ARG:HG2	G:28:LEU:HD22	0.66	1	1
K:247:ALA:HB2	K:273:ALA:HB3	0.66	1	1
B:25:MET:HE1	E:13:ALA:HB3	0.65	1	1
A:60:HIS:HB3	I:3:ARG:HH21	0.65	1	1
A:63:LYS:HG2	I:3:ARG:NE	0.65	1	1
J:99:THR:HA	J:103:ASN:HB2	0.65	1	1
C:14:VAL:HG21	D:69:GLN:HB3	0.64	1	1
K:291:PHE:HB3	K:325:LYS:HB3	0.64	1	1
J:34:ARG:HB2	J:35:PRO:HD3	0.64	1	1
A:63:LYS:CD	I:3:ARG:HA	0.63	1	1
C:4:LEU:HD12	D:82:VAL:HA	0.63	1	1
A:60:HIS:CB	I:3:ARG:HE	0.63	1	1
K:179:THR:HB	K:373:ILE:HG13	0.63	1	1
G:24:ARG:O	G:28:LEU:HG	0.62	1	1
J:355:PRO:HA	J:378:VAL:HG13	0.62	1	1
J:104:ILE:HB	J:105:PRO:HD3	0.62	1	1
B:64:ILE:O	B:68:LEU:HG	0.61	1	1
A:63:LYS:CG	I:3:ARG:NE	0.61	1	1
D:341:ASP:HA	D:376:ASP:HB2	0.61	1	1
K:330:HIS:O	K:354:ILE:HA	0.61	1	1
J:243:SER:HA	J:274:VAL:HB	0.61	1	1
J:268:HIS:HB3	J:289:ARG:HG3	0.60	1	1
A:20:SER:HB2	H:26:PRO:HB3	0.60	1	1
A:60:HIS:HB2	I:3:ARG:NE	0.60	1	1
J:316:MET:HG3	J:348:ASN:HB2	0.60	1	1
C:15:PRO:HD2	C:18:PHE:HB3	0.60	1	1
E:236:GLU:HG2	E:246:THR:HG23	0.60	1	1
F:9:LYS:HG3	F:10:GLU:OE1	0.59	1	1
K:302:TRP:HB3	K:315:GLU:HA	0.59	1	1
E:53:LEU:HD12	J:127:SER:HB3	0.59	1	1
F:6:LYS:HB2	F:48:THR:HG21	0.59	1	1
K:245:SER:HB2	K:273:ALA:HB2	0.59	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:60:HIS:CB	I:3:ARG:NE	0.59	1	1
H:28:GLU:HG3	L:29:SER:HB3	0.59	1	1
D:81:VAL:HG13	D:82:VAL:HG23	0.58	1	1

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	Analysed	Favored	Allowed	Outliers
1	2226	2036	164	26

There are 26 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	56	HIS	1
B	8	PRO	1
C	14	VAL	1
D	83	ASN	1
D	103	ASN	1
D	200	ASP	1
D	271	GLY	1
D	350	CYS	1
E	56	ASN	1
E	147	GLY	1
E	326	CYS	1
E	329	GLY	1
E	359	TRP	1
G	8	PRO	1
G	169	PRO	1
G	170	SER	1
J	81	VAL	1
J	85	TYR	1
J	200	ASP	1
J	262	GLY	1
J	292	ALA	1
J	350	CYS	1
K	56	ASN	1
K	147	GLY	1

Chain	Res	Type	Models (Total)
K	185	LEU	1
K	326	CYS	1

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric 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	1571	219	192

There are 192 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	2	GLU	1
A	3	SER	1
A	15	SER	1
A	21	SER	1
A	23	SER	1
A	29	SER	1
A	38	THR	1
A	49	GLU	1
A	52	SER	1
A	53	GLU	1
A	61	SER	1
B	10	CYS	1
B	13	GLU	1
B	14	ASP	1
B	18	LYS	1
B	34	GLN	1
B	45	ASN	1
B	47	LEU	1
B	58	HIS	1
B	86	SER	1
B	140	SER	1
B	146	GLU	1
B	158	GLN	1

Chain	Res	Type	Models (Total)
B	166	ASP	1
C	4	LEU	1
C	8	LYS	1
C	14	VAL	1
C	20	SER	1
D	21	THR	1
D	31	GLN	1
D	53	THR	1
D	63	LEU	1
D	65	LYS	1
D	72	GLN	1
D	77	ASP	1
D	78	ASN	1
D	83	ASN	1
D	86	SER	1
D	87	SER	1
D	89	LEU	1
D	92	HIS	1
D	99	THR	1
D	106	THR	1
D	124	LYS	1
D	125	LEU	1
D	153	GLU	1
D	156	GLU	1
D	163	GLU	1
D	164	THR	1
D	174	SER	1
D	175	SER	1
D	213	LYS	1
D	223	THR	1
D	245	LEU	1
D	259	ASP	1
D	291	THR	1
D	319	SER	1
D	330	THR	1

Chain	Res	Type	Models (Total)
D	335	LYS	1
D	336	GLN	1
D	366	THR	1
D	371	LYS	1
D	374	THR	1
D	376	ASP	1
D	386	SER	1
D	397	ILE	1
D	400	PHE	1
E	9	THR	1
E	18	THR	1
E	28	GLN	1
E	60	SER	1
E	80	ILE	1
E	89	THR	1
E	124	GLU	1
E	129	THR	1
E	139	ASP	1
E	170	GLU	1
E	172	ASP	1
E	174	SER	1
E	182	GLN	1
E	185	LEU	1
E	188	SER	1
E	208	THR	1
E	210	THR	1
E	241	ASN	1
E	243	ARG	1
E	257	GLU	1
E	284	ASP	1
E	287	SER	1
E	301	THR	1
E	304	ASN	1
E	310	GLU	1
E	319	SER	1

Chain	Res	Type	Models (Total)
E	346	THR	1
E	351	ASP	1
E	358	THR	1
E	377	ASN	1
E	380	THR	1
F	1	LYS	1
F	13	THR	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*".

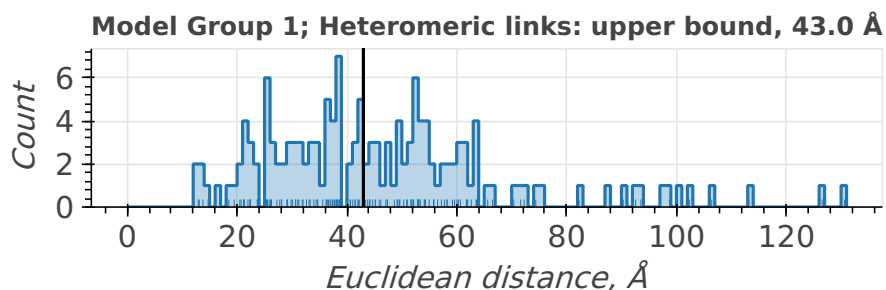
Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

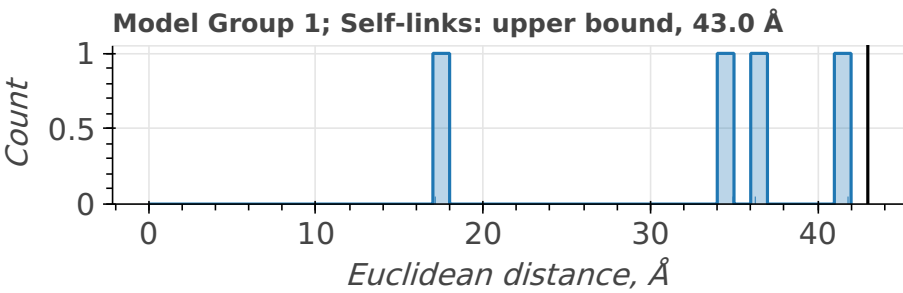
There are 156 crosslinking restraints combined in 156 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	43.0	156

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.





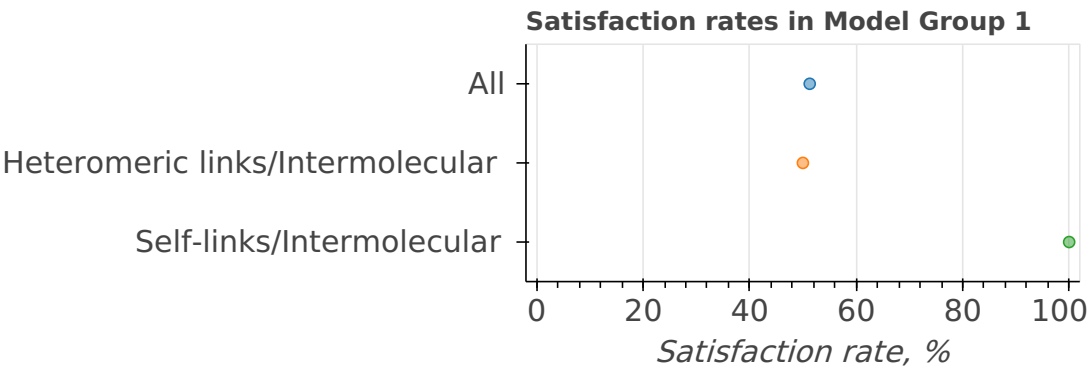
Satisfaction of restraints

Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=156)
1	1	1	1/1	All	51.28	48.72	156
				Heteromeric links/ Intermolecular	50.00	50.00	152
				Self-links/ Intermolecular	100.00	0.00	4

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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