



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:26 AM UTC

PDB ID : 1LSG / pdb_00001lsg
Title : THREE-DIMENSIONAL STRUCTURE OF THE PLATELET INTEGRIN RECOGNITION SEGMENT OF THE FIBRINOGEN GAMMA CHAIN OBTAINED BY CARRIER PROTEIN-DRIVEN CRYSTALLIZATION
Authors : Patel, H.; Anderson, W.F.
Deposited on : 1994-10-25
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

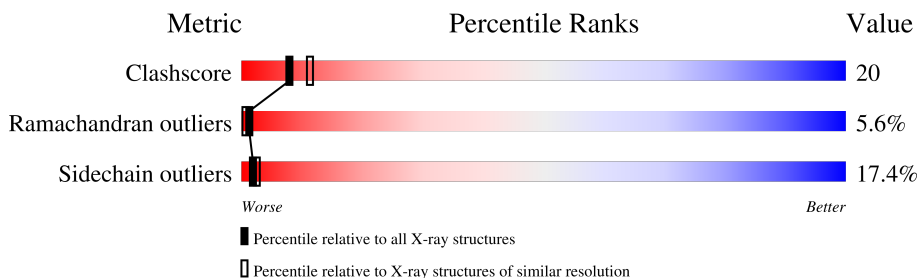
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	144	36% 42% 15% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1110 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 HEN EGG WHITE LYSOZYME.

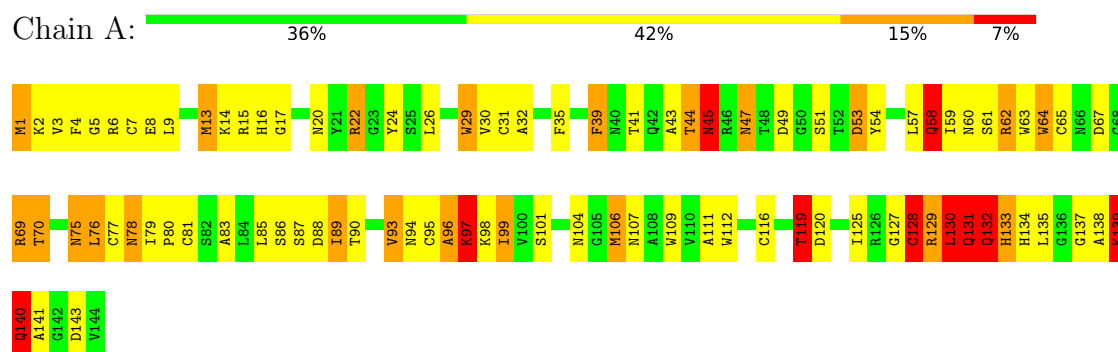
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	144	1110	678	216	205	11	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.90Å 74.00Å 30.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1110	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.54	9/1132 (0.8%)	2.78	108/1527 (7.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	HIS	CD2-NE2	-7.19	1.29	1.37
1	A	89	ILE	CA-CB	7.13	1.64	1.54
1	A	133	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	16	HIS	CG-ND1	-5.97	1.31	1.38
1	A	125	ILE	CA-CB	5.91	1.62	1.54
1	A	112	TRP	CG-CD2	-5.63	1.33	1.43
1	A	133	HIS	CG-ND1	-5.58	1.32	1.38
1	A	53	ASP	CA-CB	-5.27	1.46	1.53
1	A	134	HIS	CD2-NE2	-5.18	1.32	1.37

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLN	N-CA-C	18.51	137.90	112.72
1	A	138	ALA	N-CA-C	17.91	134.70	110.35
1	A	139	LYS	N-CA-C	10.67	133.53	110.80
1	A	3	VAL	N-CA-C	-10.49	93.36	108.36
1	A	140	GLN	OE1-CD-NE2	-10.47	112.13	122.60
1	A	15	ARG	CA-CB-CG	10.02	134.15	114.10
1	A	49	ASP	CA-CB-CG	9.92	122.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	62	ARG	N-CA-C	-9.30	100.71	111.03
1	A	138	ALA	CA-C-N	9.10	138.93	121.54
1	A	138	ALA	C-N-CA	9.10	138.93	121.54
1	A	78	ASN	OD1-CG-ND2	-8.49	114.11	122.60
1	A	47	ASN	CA-CB-CG	8.34	120.94	112.60
1	A	44	THR	CA-CB-OG1	-8.28	97.18	109.60
1	A	64	TRP	N-CA-C	8.07	123.41	112.68
1	A	132	GLN	CA-CB-CG	8.05	130.21	114.10
1	A	130	LEU	N-CA-C	-8.04	93.66	110.80
1	A	138	ALA	CA-C-O	7.93	129.95	121.55
1	A	112	TRP	CA-C-O	-7.82	112.85	120.90
1	A	6	ARG	N-CA-C	7.64	123.98	111.37
1	A	132	GLN	N-CA-C	7.52	120.54	111.82
1	A	140	GLN	CA-CB-CG	-7.51	99.08	114.10
1	A	128	CYS	CA-CB-SG	7.50	131.64	114.40
1	A	138	ALA	O-C-N	7.45	131.97	122.81
1	A	140	GLN	CG-CD-NE2	7.44	127.56	116.40
1	A	58	GLN	OE1-CD-NE2	-7.42	115.18	122.60
1	A	104	ASN	CA-CB-CG	7.36	119.96	112.60
1	A	88	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	134	HIS	N-CA-C	-7.18	98.11	109.23
1	A	106	MET	N-CA-C	7.13	123.21	113.37
1	A	58	GLN	CG-CD-NE2	7.02	126.93	116.40
1	A	44	THR	CA-CB-CG2	6.86	122.16	110.50
1	A	45	ASN	CA-C-O	-6.82	113.02	120.24
1	A	59	ILE	N-CA-CB	-6.71	103.44	110.95
1	A	63	TRP	N-CA-C	6.71	121.69	112.90
1	A	143	ASP	N-CA-CB	6.69	120.01	109.71
1	A	129	ARG	CB-CG-CD	6.64	126.58	111.30
1	A	26	LEU	CB-CA-C	-6.53	100.00	110.84
1	A	131	GLN	CB-CG-CD	6.51	123.66	112.60
1	A	107	ASN	CA-CB-CG	6.49	119.09	112.60
1	A	128	CYS	N-CA-C	6.47	120.05	109.24
1	A	119	THR	CA-CB-CG2	6.47	121.50	110.50
1	A	139	LYS	O-C-N	-6.45	114.01	122.59
1	A	83	ALA	N-CA-C	-6.43	104.36	111.82
1	A	119	THR	N-CA-C	-6.41	100.72	110.14
1	A	70	THR	CA-C-N	6.39	127.36	120.13
1	A	70	THR	C-N-CA	6.39	127.36	120.13
1	A	58	GLN	N-CA-CB	-6.36	102.52	111.62
1	A	129	ARG	CA-CB-CG	-6.36	101.39	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	1	MET	CA-CB-CG	6.26	126.63	114.10
1	A	133	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	A	96	ALA	O-C-N	-6.23	115.66	122.07
1	A	140	GLN	N-CA-CB	-6.22	100.08	110.22
1	A	13	MET	N-CA-C	-6.20	104.41	112.23
1	A	101	SER	CA-C-O	6.20	127.85	120.53
1	A	104	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	5	GLY	N-CA-C	-6.12	99.81	110.71
1	A	15	ARG	O-C-N	-6.11	114.46	122.59
1	A	143	ASP	O-C-N	5.97	130.49	122.96
1	A	99	ILE	N-CA-C	-5.89	104.99	110.53
1	A	69	ARG	CB-CG-CD	-5.87	97.80	111.30
1	A	32	ALA	CA-C-O	-5.86	114.66	120.70
1	A	98	LYS	N-CA-C	-5.84	106.77	114.31
1	A	139	LYS	CA-C-N	-5.81	111.34	122.61
1	A	139	LYS	C-N-CA	-5.81	111.34	122.61
1	A	22	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	A	101	SER	CA-CB-OG	-5.79	99.53	111.10
1	A	22	ARG	N-CA-C	5.77	123.09	110.80
1	A	30	VAL	CA-C-N	5.77	129.07	120.31
1	A	30	VAL	C-N-CA	5.77	129.07	120.31
1	A	77	CYS	CA-CB-SG	-5.76	101.14	114.40
1	A	143	ASP	N-CA-C	-5.73	101.17	109.59
1	A	97	LYS	CA-C-N	5.70	131.19	122.24
1	A	97	LYS	C-N-CA	5.70	131.19	122.24
1	A	133	HIS	N-CA-C	5.68	118.94	111.28
1	A	78	ASN	N-CA-C	-5.67	103.93	111.02
1	A	26	LEU	N-CA-C	5.64	120.61	111.37
1	A	129	ARG	N-CA-C	-5.63	108.20	114.62
1	A	63	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	A	60	ASN	N-CA-C	5.59	118.34	110.23
1	A	44	THR	N-CA-C	-5.55	98.97	110.80
1	A	127	GLY	N-CA-C	-5.54	107.36	115.72
1	A	61	SER	N-CA-C	5.51	119.99	113.16
1	A	49	ASP	O-C-N	-5.49	115.80	122.22
1	A	64	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	A	29	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	A	58	GLN	N-CA-C	5.42	118.67	111.30
1	A	131	GLN	O-C-N	-5.41	115.39	122.59
1	A	112	TRP	CG-CD1-NE1	-5.41	103.17	110.20
1	A	112	TRP	CE2-CD2-CE3	5.40	124.20	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	131	GLN	CG-CD-NE2	5.27	124.30	116.40
1	A	139	LYS	N-CA-CB	-5.25	101.61	110.49
1	A	64	TRP	CD2-CE2-CZ2	-5.22	117.18	122.40
1	A	87	SER	N-CA-C	5.16	119.43	113.18
1	A	29	TRP	CD1-CG-CD2	5.16	114.55	106.30
1	A	119	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	130	LEU	CA-CB-CG	5.13	134.26	116.30
1	A	120	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	64	TRP	CD1-CG-CD2	5.11	114.48	106.30
1	A	17	GLY	O-C-N	-5.09	115.97	122.43
1	A	67	ASP	CA-C-O	5.08	124.72	119.14
1	A	79	ILE	CA-C-N	5.08	125.07	119.89
1	A	79	ILE	C-N-CA	5.08	125.07	119.89
1	A	75	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	63	TRP	CD1-CG-CD2	5.03	114.35	106.30
1	A	90	THR	N-CA-CB	-5.03	102.45	109.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	CYS	Peptide

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	1110	0	1070	40	0
All	All	1110	0	1070	40	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 20.

All (40) 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:31:CYS:SG	1:A:116:CYS:SG	2.56	0.87
1:A:31:CYS:HG	1:A:116:CYS:HG	0.79	0.78
1:A:53:ASP:HB3	1:A:58:GLN:HG3	1.74	0.69
1:A:99:ILE:HD12	1:A:109:TRP:CZ2	2.29	0.68
1:A:75:ASN:ND2	1:A:78:ASN:HA	2.11	0.64
1:A:93:VAL:O	1:A:97:LYS:HG2	1.99	0.62
1:A:9:LEU:HD22	1:A:39:PHE:CD1	2.37	0.60
1:A:9:LEU:HD11	1:A:13:MET:HE3	1.84	0.60
1:A:140:GLN:HE21	1:A:140:GLN:HA	1.71	0.55
1:A:31:CYS:CB	1:A:116:CYS:HG	2.20	0.54
1:A:4:PHE:HB2	1:A:39:PHE:HB3	1.90	0.54
1:A:140:GLN:HA	1:A:140:GLN:NE2	2.21	0.53
1:A:75:ASN:HD21	1:A:78:ASN:HA	1.72	0.53
1:A:2:LYS:HE2	1:A:4:PHE:CZ	2.44	0.53
1:A:106:MET:HG2	1:A:109:TRP:CZ3	2.44	0.53
1:A:64:TRP:CZ3	1:A:76:LEU:HD12	2.44	0.53
1:A:62:ARG:HA	1:A:70:THR:HG21	1.91	0.52
1:A:116:CYS:O	1:A:119:THR:HB	2.11	0.51
1:A:132:GLN:O	1:A:133:HIS:ND1	2.45	0.50
1:A:2:LYS:HG2	1:A:4:PHE:CE1	2.48	0.49
1:A:24:TYR:HB2	1:A:29:TRP:HE1	1.79	0.48
1:A:31:CYS:SG	1:A:116:CYS:CB	3.01	0.48
1:A:96:ALA:HA	1:A:99:ILE:HG13	1.98	0.46
1:A:8:GLU:HA	1:A:130:LEU:HD22	1.98	0.46
1:A:64:TRP:HZ3	1:A:76:LEU:HD12	1.81	0.46
1:A:35:PHE:HB3	1:A:111:ALA:HB1	1.98	0.45
1:A:139:LYS:HD2	1:A:140:GLN:HG2	1.98	0.45
1:A:97:LYS:HB3	1:A:97:LYS:HE2	1.76	0.43
1:A:106:MET:HG2	1:A:109:TRP:CE3	2.54	0.43
1:A:43:ALA:HB3	1:A:58:GLN:HE22	1.84	0.43
1:A:64:TRP:CZ2	1:A:99:ILE:HG23	2.54	0.42
1:A:95:CYS:O	1:A:99:ILE:HG13	2.18	0.42
1:A:65:CYS:HB2	1:A:81:CYS:HA	2.02	0.42
1:A:128:CYS:H	1:A:137:GLY:HA3	1.84	0.42
1:A:31:CYS:C	1:A:116:CYS:SG	3.03	0.41
1:A:7:CYS:HB2	1:A:131:GLN:OE1	2.20	0.41
1:A:132:GLN:OE1	1:A:133:HIS:N	2.54	0.41
1:A:54:TYR:CD2	1:A:85:LEU:HD11	2.56	0.40
1:A:45:ASN:HB2	1:A:53:ASP:HB2	2.03	0.40
1:A:99:ILE:HD12	1:A:109:TRP:HZ2	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	142/144 (99%)	109 (77%)	25 (18%)	8 (6%)	1 1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	139	LYS
1	A	20	ASN
1	A	141	ALA
1	A	97	LYS
1	A	131	GLN
1	A	135	LEU
1	A	41	THR

5.3.2 Protein sidechains [i](#)

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	115/115 (100%)	95 (83%)	20 (17%)	2 2

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	LYS
1	A	44	THR

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Mol	Chain	Res	Type
1	A	45	ASN
1	A	47	ASN
1	A	51	SER
1	A	57	LEU
1	A	58	GLN
1	A	69	ARG
1	A	76	LEU
1	A	80	PRO
1	A	86	SER
1	A	89	ILE
1	A	93	VAL
1	A	119	THR
1	A	129	ARG
1	A	130	LEU
1	A	132	GLN
1	A	139	LYS
1	A	140	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	45	ASN
1	A	47	ASN
1	A	58	GLN
1	A	114	ASN
1	A	140	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.