



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:11 AM UTC

PDB ID : 1IC5 / pdb_00001ic5
Title : CRYSTAL STRUCTURE OF HYHEL-10 FV MUTANT(HD99A)-HEN
LYSOZYME COMPLEX
Authors : Shiroishi, M.; Yokota, A.; Tsumoto, K.; Kondo, H.; Nishimiya, Y.; Horii, K.;
Matsushima, M.; Ogasahara, K.; Yutani, K.; Kumagai, I.
Deposited on : 2001-03-30
Resolution : 2.30 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 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

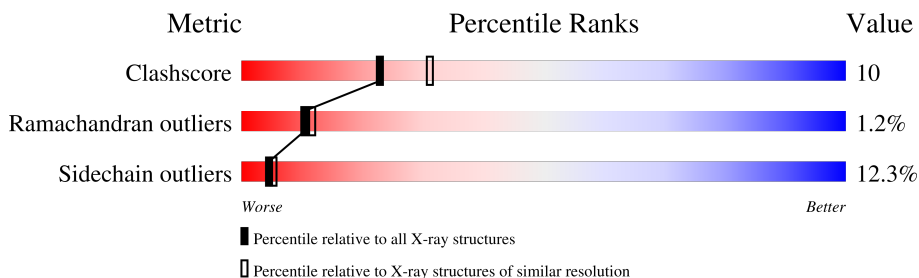
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	L	107	50% 32% 12% 6%
2	H	114	60% 32% 7% .
3	Y	129	51% 35% 9% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2834 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 LYSOZYME BINDING IG KAPPA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	107	Total	C	N	O	S	0	0	0
			818	511	138	166	3			

- Molecule 2 is a protein called IGG1 FAB CHAIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	114	Total	C	N	O	S	0	0	0
			899	566	144	186	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	99	ALA	ASP	engineered mutation	UNP P01823

- Molecule 3 is a protein called LYSOZYME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	35	Total	O	0	0
			35	35		
4	H	37	Total	O	0	0
			37	37		
4	Y	44	Total	O	0	0
			44	44		

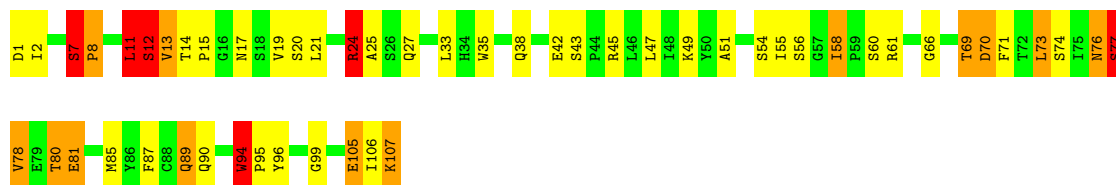
3 Residue-property plots [i](#)

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: LYSOZYME BINDING IG KAPPA CHAIN

Chain L: 



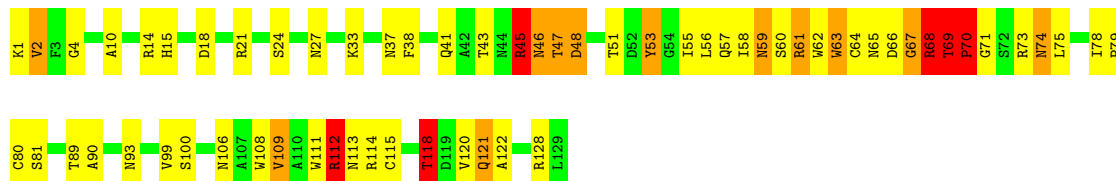
• Molecule 2: IGG1 FAB CHAIN H

Chain H: 



• Molecule 3: LYSOZYME C

Chain Y: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.00Å 57.00Å 238.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2834	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	L	1.20	0/837	2.54	62/1133 (5.5%)
2	H	1.21	0/922	2.29	44/1259 (3.5%)
3	Y	1.22	1/1021 (0.1%)	2.45	83/1379 (6.0%)
All	All	1.21	1/2780 (0.0%)	2.42	189/3771 (5.0%)

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	L	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	4	GLY	N-CA	5.49	1.52	1.45

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	71	ARG	CD-NE-CZ	15.91	146.68	124.40
1	L	94	TRP	CA-C-O	-14.18	105.24	120.70
1	L	69	THR	N-CA-CB	-12.42	94.38	110.90
1	L	49	LYS	CA-CB-CG	12.24	138.57	114.10
1	L	7	SER	CA-C-O	-12.05	103.66	120.16
3	Y	2	VAL	N-CA-CB	10.46	125.08	111.90
1	L	70	ASP	CA-CB-CG	-10.43	102.17	112.60
3	Y	121	GLN	CB-CG-CD	9.90	129.44	112.60
2	H	111	VAL	CA-C-O	-9.09	110.81	120.53
2	H	51	VAL	CB-CA-C	-8.80	97.44	110.81
3	Y	74	ASN	OD1-CG-ND2	-8.63	113.97	122.60
1	L	81	GLU	CB-CG-CD	8.46	126.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	111	VAL	O-C-N	8.11	132.59	123.10
3	Y	4	GLY	CA-C-N	8.10	130.97	120.44
3	Y	4	GLY	C-N-CA	8.10	130.97	120.44
3	Y	15	HIS	CA-CB-CG	-7.82	105.98	113.80
3	Y	41	GLN	OE1-CD-NE2	7.65	130.25	122.60
1	L	1	ASP	CA-CB-CG	-7.65	104.95	112.60
2	H	44	ARG	CD-NE-CZ	7.63	135.08	124.40
1	L	54	SER	O-C-N	-7.59	114.20	122.85
1	L	54	SER	CA-CB-OG	-7.58	95.94	111.10
2	H	101	ASP	CA-C-O	-7.57	112.91	120.70
1	L	56	SER	CA-C-O	-7.53	113.56	121.55
2	H	43	ASN	OD1-CG-ND2	7.40	130.00	122.60
3	Y	4	GLY	N-CA-C	-7.38	102.63	112.82
3	Y	118	THR	N-CA-CB	-7.35	99.74	110.70
1	L	8	PRO	CA-N-CD	-7.30	101.78	112.00
2	H	3	GLN	O-C-N	-7.26	114.42	123.27
3	Y	63	TRP	N-CA-C	7.20	122.12	113.12
2	H	97	ASN	CA-CB-CG	7.17	119.77	112.60
3	Y	59	ASN	CA-C-O	7.12	129.16	121.05
3	Y	57	GLN	CA-C-N	7.08	130.61	120.98
3	Y	57	GLN	C-N-CA	7.08	130.61	120.98
3	Y	74	ASN	CB-CG-ND2	6.99	126.88	116.40
1	L	69	THR	OG1-CB-CG2	6.98	123.26	109.30
3	Y	90	ALA	CA-C-N	6.97	129.62	120.28
3	Y	90	ALA	C-N-CA	6.97	129.62	120.28
3	Y	45	ARG	CB-CA-C	6.97	121.23	109.80
3	Y	60	SER	CA-C-O	-6.96	110.82	119.38
1	L	61	ARG	NE-CZ-NH2	6.94	125.45	119.20
2	H	73	THR	N-CA-CB	-6.93	99.53	110.28
1	L	80	THR	N-CA-CB	6.86	120.92	110.28
3	Y	106	ASN	CA-CB-CG	-6.82	105.78	112.60
3	Y	108	TRP	CA-C-N	6.80	129.77	120.46
3	Y	108	TRP	C-N-CA	6.80	129.77	120.46
3	Y	18	ASP	CA-CB-CG	-6.73	105.87	112.60
3	Y	120	VAL	CA-C-O	-6.71	113.22	120.47
1	L	60	SER	CA-CB-OG	-6.69	97.73	111.10
3	Y	61	ARG	O-C-N	-6.67	114.54	122.15
3	Y	112	ARG	CD-NE-CZ	6.67	133.73	124.40
2	H	43	ASN	CA-CB-CG	-6.65	105.95	112.60
3	Y	109	VAL	CA-C-O	-6.65	114.04	120.95
3	Y	45	ARG	CB-CG-CD	6.64	126.58	111.30
1	L	73	LEU	CA-C-O	-6.63	113.02	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	15	SER	CA-C-N	-6.62	110.46	122.12
2	H	15	SER	C-N-CA	-6.62	110.46	122.12
3	Y	24	SER	CA-C-N	6.59	129.41	120.38
3	Y	24	SER	C-N-CA	6.59	129.41	120.38
2	H	104	GLY	N-CA-C	-6.54	101.90	112.31
2	H	3	GLN	CB-CG-CD	6.54	123.72	112.60
3	Y	93	ASN	CB-CG-OD1	6.53	133.86	120.80
3	Y	111	TRP	CA-C-O	-6.51	113.52	120.42
1	L	45	ARG	CD-NE-CZ	6.48	133.47	124.40
3	Y	69	THR	CA-C-O	6.45	126.55	119.32
1	L	56	SER	CA-CB-OG	-6.45	98.21	111.10
3	Y	10	ALA	O-C-N	-6.43	115.30	122.12
1	L	2	ILE	N-CA-C	6.43	118.06	108.54
1	L	56	SER	CB-CA-C	-6.43	98.11	109.62
2	H	41	PRO	CA-C-O	-6.42	108.92	120.60
1	L	27	GLN	CB-CG-CD	6.41	123.50	112.60
2	H	76	ASN	O-C-N	-6.34	114.10	122.47
1	L	8	PRO	N-CA-CB	6.34	109.91	103.25
3	Y	128	ARG	NE-CZ-NH1	-6.32	115.18	121.50
2	H	41	PRO	O-C-N	-6.32	114.11	122.64
3	Y	112	ARG	CA-C-O	-6.29	113.88	120.55
2	H	47	TYR	CA-C-O	-6.25	113.24	120.49
1	L	54	SER	N-CA-CB	-6.24	100.97	110.45
2	H	71	ARG	NE-CZ-NH1	-6.22	115.28	121.50
3	Y	64	CYS	CA-C-N	-6.16	114.42	123.05
3	Y	64	CYS	C-N-CA	-6.16	114.42	123.05
3	Y	65	ASN	CA-C-O	-6.15	113.56	120.32
3	Y	111	TRP	N-CA-C	-6.14	104.67	111.36
1	L	81	GLU	CA-CB-CG	6.13	126.36	114.10
3	Y	38	PHE	CA-CB-CG	6.13	119.93	113.80
3	Y	89	THR	CA-CB-OG1	-6.13	100.41	109.60
3	Y	45	ARG	O-C-N	-6.12	116.24	123.22
2	H	64	LYS	CA-CB-CG	-6.12	101.86	114.10
3	Y	57	GLN	O-C-N	-6.09	115.37	122.86
1	L	12	SER	CA-C-N	-6.08	114.54	122.51
1	L	12	SER	C-N-CA	-6.08	114.54	122.51
3	Y	112	ARG	CB-CA-C	-6.07	100.71	110.79
3	Y	128	ARG	CA-C-N	-6.05	110.80	121.70
3	Y	128	ARG	C-N-CA	-6.05	110.80	121.70
1	L	94	TRP	CB-CA-C	6.05	119.01	109.27
1	L	45	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	L	55	ILE	N-CA-CB	-6.01	102.75	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	24	SER	CA-CB-OG	-6.00	99.10	111.10
3	Y	65	ASN	CA-CB-CG	5.99	118.59	112.60
2	H	15	SER	CA-CB-OG	-5.98	99.13	111.10
2	H	95	CYS	N-CA-CB	5.98	120.37	110.63
3	Y	122	ALA	N-CA-C	-5.97	104.84	111.71
1	L	94	TRP	O-C-N	-5.95	114.98	121.53
3	Y	93	ASN	CB-CG-ND2	-5.95	107.47	116.40
3	Y	68	ARG	CA-C-N	-5.88	112.66	121.83
3	Y	68	ARG	C-N-CA	-5.88	112.66	121.83
1	L	99	GLY	N-CA-C	-5.87	104.72	112.82
2	H	4	LEU	CA-C-O	-5.86	114.37	120.70
1	L	87	PHE	CA-CB-CG	5.84	119.64	113.80
1	L	24	ARG	NE-CZ-NH2	5.83	124.44	119.20
3	Y	27	ASN	CA-C-N	5.82	128.08	120.28
3	Y	27	ASN	C-N-CA	5.82	128.08	120.28
2	H	35	SER	N-CA-CB	-5.81	102.21	111.62
3	Y	67	GLY	O-C-N	-5.77	115.20	122.70
3	Y	71	GLY	CA-C-N	5.76	129.55	121.02
3	Y	71	GLY	C-N-CA	5.76	129.55	121.02
2	H	77	GLN	CA-C-O	-5.76	114.90	121.58
1	L	47	LEU	CA-C-N	5.73	130.96	122.71
1	L	47	LEU	C-N-CA	5.73	130.96	122.71
1	L	96	TYR	N-CA-CB	5.72	118.38	109.97
3	Y	118	THR	CA-CB-OG1	5.72	118.17	109.60
3	Y	65	ASN	OD1-CG-ND2	-5.70	116.90	122.60
3	Y	118	THR	N-CA-C	-5.70	101.76	110.14
1	L	66	GLY	CA-C-O	-5.69	118.03	122.52
1	L	71	PHE	CA-CB-CG	-5.68	108.12	113.80
3	Y	114	ARG	NH1-CZ-NH2	5.68	126.68	119.30
3	Y	114	ARG	CB-CG-CD	-5.67	98.25	111.30
3	Y	47	THR	N-CA-CB	5.66	118.37	109.94
1	L	76	ASN	O-C-N	-5.63	116.45	123.04
3	Y	33	LYS	CA-C-O	-5.62	114.92	120.82
3	Y	121	GLN	CG-CD-NE2	-5.59	108.01	116.40
1	L	51	ALA	CA-C-O	-5.55	112.57	120.51
2	H	111	VAL	CA-C-N	-5.55	111.47	121.62
2	H	111	VAL	C-N-CA	-5.55	111.47	121.62
1	L	43	SER	N-CA-CB	-5.54	102.07	110.05
3	Y	41	GLN	CG-CD-OE1	-5.54	109.72	120.80
1	L	70	ASP	O-C-N	-5.52	116.87	123.27
1	L	105	GLU	CA-C-N	5.51	128.82	120.77
1	L	105	GLU	C-N-CA	5.51	128.82	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	SER	N-CA-CB	5.51	121.76	111.52
2	H	33	TYR	N-CA-C	-5.51	101.19	109.95
2	H	73	THR	CB-CA-C	5.51	121.24	110.67
1	L	11	LEU	CA-C-N	-5.48	114.99	122.93
1	L	11	LEU	C-N-CA	-5.48	114.99	122.93
1	L	61	ARG	CA-C-O	-5.47	112.88	119.49
3	Y	113	ASN	CA-C-O	-5.46	112.88	119.27
1	L	42	GLU	CA-C-O	5.45	127.38	121.06
1	L	105	GLU	O-C-N	-5.44	117.12	123.27
3	Y	53	TYR	N-CA-C	5.43	117.75	108.90
1	L	69	THR	CA-C-O	5.42	124.79	118.77
1	L	58	ILE	CA-CB-CG1	-5.42	101.19	110.40
2	H	57	THR	CA-C-N	5.42	130.41	122.77
2	H	57	THR	C-N-CA	5.42	130.41	122.77
2	H	19	SER	CA-C-N	-5.40	114.11	122.59
2	H	19	SER	C-N-CA	-5.40	114.11	122.59
2	H	10	SER	N-CA-CB	-5.39	102.73	110.65
1	L	1	ASP	CB-CG-OD2	-5.38	106.03	118.40
3	Y	2	VAL	CB-CA-C	5.36	117.96	110.99
1	L	1	ASP	OD1-CG-OD2	5.35	135.75	122.90
2	H	34	TRP	CA-C-N	-5.32	113.84	122.36
2	H	34	TRP	C-N-CA	-5.32	113.84	122.36
3	Y	46	ASN	N-CA-C	5.30	118.30	110.46
1	L	60	SER	CB-CA-C	-5.30	99.15	110.32
2	H	62	SER	O-C-N	-5.30	115.50	122.39
1	L	7	SER	CA-CB-OG	-5.28	100.53	111.10
1	L	24	ARG	CB-CG-CD	5.27	123.43	111.30
3	Y	100	SER	CA-CB-OG	-5.27	100.56	111.10
1	L	106	ILE	O-C-N	-5.26	117.03	122.66
3	Y	1	LYS	CA-C-N	-5.26	116.09	123.13
3	Y	1	LYS	C-N-CA	-5.26	116.09	123.13
2	H	51	VAL	CA-C-O	-5.25	114.74	120.72
3	Y	58	ILE	O-C-N	-5.24	116.96	122.67
1	L	89	GLN	CA-C-O	-5.24	114.31	120.60
1	L	81	GLU	CA-C-N	5.24	131.80	122.06
1	L	81	GLU	C-N-CA	5.24	131.80	122.06
3	Y	128	ARG	CB-CA-C	-5.24	101.31	109.84
3	Y	37	ASN	CA-CB-CG	-5.22	107.38	112.60
1	L	90	GLN	OE1-CD-NE2	-5.21	117.39	122.60
2	H	40	PHE	CA-CB-CG	-5.21	108.59	113.80
3	Y	68	ARG	NE-CZ-NH1	-5.18	116.32	121.50
3	Y	69	THR	N-CA-C	5.14	116.85	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	29	ILE	O-C-N	-5.14	115.32	122.05
3	Y	118	THR	OG1-CB-CG2	5.10	119.50	109.30
2	H	71	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	L	20	SER	CA-CB-OG	-5.07	100.95	111.10
3	Y	90	ALA	O-C-N	-5.07	116.82	122.09
2	H	44	ARG	CB-CA-C	5.05	118.08	109.75
3	Y	109	VAL	CA-CB-CG1	5.04	118.97	110.40
3	Y	112	ARG	N-CA-CB	5.02	117.50	110.12
3	Y	111	TRP	N-CA-CB	5.01	117.58	110.16

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	33	LEU	Mainchain
1	L	7	SER	Peptide,Mainchain
1	L	94	TRP	Peptide,Mainchain

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	L	818	0	784	16	0
2	H	899	0	846	13	0
3	Y	1001	0	959	27	0
4	H	37	0	0	1	0
4	L	35	0	0	0	0
4	Y	44	0	0	2	0
All	All	2834	0	2589	55	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 10.

All (55) 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)
3:Y:61:ARG:HH12	3:Y:70:PRO:HB2	1.25	1.02
3:Y:74:ASN:HD21	3:Y:78:ILE:H	1.14	0.94
1:L:12:SER:HB2	1:L:107:LYS:HB2	1.61	0.81
3:Y:59:ASN:ND2	3:Y:61:ARG:H	1.85	0.75
3:Y:78:ILE:HG13	3:Y:79:PRO:HD2	1.73	0.71
2:H:42:GLY:O	2:H:43:ASN:HB2	1.91	0.69
3:Y:109:VAL:HG22	3:Y:112:ARG:NH2	2.08	0.69
3:Y:45:ARG:HD3	3:Y:68:ARG:HH22	1.62	0.65
1:L:38:GLN:OE1	2:H:39:LYS:HE3	1.98	0.63
3:Y:61:ARG:NH1	3:Y:70:PRO:HB2	2.08	0.60
3:Y:45:ARG:HG3	3:Y:51:THR:OG1	2.02	0.59
3:Y:74:ASN:HD21	3:Y:78:ILE:N	1.93	0.59
3:Y:118:THR:CG2	4:Y:134:HOH:O	2.51	0.58
2:H:34:TRP:HB3	2:H:78:TYR:CZ	2.38	0.57
3:Y:118:THR:HG21	4:Y:134:HOH:O	2.03	0.57
2:H:13:LYS:HE3	2:H:114:ALA:H	1.69	0.57
1:L:12:SER:HA	1:L:105:GLU:O	2.09	0.53
3:Y:66:ASP:OD1	3:Y:69:THR:OG1	2.21	0.53
3:Y:45:ARG:HD3	3:Y:68:ARG:NH2	2.23	0.53
3:Y:74:ASN:ND2	3:Y:78:ILE:H	1.96	0.53
1:L:17:ASN:O	1:L:78:VAL:HG13	2.10	0.51
3:Y:115:CYS:O	3:Y:118:THR:HB	2.10	0.51
2:H:64:LYS:O	2:H:65:SER:HB2	2.11	0.51
2:H:51:VAL:HG22	2:H:69:ILE:HG21	1.92	0.51
1:L:94:TRP:CD2	1:L:95:PRO:HA	2.47	0.50
2:H:51:VAL:HG22	2:H:69:ILE:CG2	2.43	0.48
1:L:7:SER:OG	1:L:8:PRO:N	2.45	0.48
2:H:60:ASN:HB3	2:H:63:LEU:HD22	1.95	0.48
1:L:13:VAL:HG21	1:L:19:VAL:CG1	2.44	0.48
2:H:72:ASP:OD2	2:H:75:LYS:HE3	2.13	0.48
3:Y:66:ASP:O	3:Y:68:ARG:N	2.46	0.48
1:L:24:ARG:HG2	1:L:25:ALA:N	2.28	0.47
1:L:76:ASN:HD22	1:L:77:SER:N	2.13	0.47
1:L:85:MET:HG3	4:H:137:HOH:O	2.15	0.46
3:Y:14:ARG:HH11	3:Y:14:ARG:HD2	1.58	0.46
3:Y:68:ARG:HH11	3:Y:68:ARG:HB2	1.80	0.46
3:Y:62:TRP:HZ3	3:Y:73:ARG:NH1	2.13	0.46
1:L:76:ASN:HD22	1:L:76:ASN:C	2.25	0.45
1:L:14:THR:O	1:L:15:PRO:C	2.58	0.45
1:L:14:THR:HG22	1:L:15:PRO:O	2.17	0.44
3:Y:53:TYR:CD2	3:Y:80:CYS:HB3	2.53	0.43
1:L:13:VAL:HG11	1:L:78:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:48:ASP:O	3:Y:61:ARG:NH2	2.51	0.43
3:Y:46:ASN:O	3:Y:47:THR:C	2.61	0.43
3:Y:68:ARG:HH11	3:Y:68:ARG:CB	2.32	0.43
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.55	0.42
3:Y:21:ARG:HA	3:Y:21:ARG:HD2	1.84	0.42
3:Y:59:ASN:ND2	3:Y:61:ARG:N	2.62	0.41
3:Y:63:TRP:CE3	3:Y:75:LEU:HB2	2.55	0.41
1:L:11:LEU:HD23	1:L:11:LEU:HA	1.91	0.41
3:Y:56:LEU:HD23	3:Y:56:LEU:HA	1.97	0.41
2:H:64:LYS:O	2:H:65:SER:CB	2.69	0.41
2:H:13:LYS:O	2:H:16:GLN:HG2	2.19	0.41
2:H:29:ILE:HD13	2:H:29:ILE:HG21	1.87	0.40
2:H:21:THR:HB	2:H:79:TYR:CD1	2.57	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	L	105/107 (98%)	100 (95%)	4 (4%)	1 (1%)	12	15
2	H	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
3	Y	127/129 (98%)	120 (94%)	4 (3%)	3 (2%)	4	4
All	All	344/350 (98%)	330 (96%)	10 (3%)	4 (1%)	10	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	70	PRO
3	Y	48	ASP
3	Y	67	GLY
1	L	77	SER

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	L	94/94 (100%)	78 (83%)	16 (17%)	2	2
2	H	101/101 (100%)	92 (91%)	9 (9%)	9	12
3	Y	105/105 (100%)	93 (89%)	12 (11%)	5	6
All	All	300/300 (100%)	263 (88%)	37 (12%)	4	5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	11	LEU
1	L	12	SER
1	L	13	VAL
1	L	21	LEU
1	L	24	ARG
1	L	58	ILE
1	L	69	THR
1	L	70	ASP
1	L	74	SER
1	L	77	SER
1	L	78	VAL
1	L	80	THR
1	L	81	GLU
1	L	89	GLN
1	L	107	LYS
2	H	11	LEU
2	H	21	THR
2	H	45	LEU
2	H	51	VAL
2	H	63	LEU
2	H	65	SER
2	H	67	ILE
2	H	73	THR
2	H	88	GLU
3	Y	2	VAL

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Mol	Chain	Res	Type
3	Y	43	THR
3	Y	45	ARG
3	Y	55	ILE
3	Y	68	ARG
3	Y	69	THR
3	Y	70	PRO
3	Y	81	SER
3	Y	99	VAL
3	Y	112	ARG
3	Y	118	THR
3	Y	121	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	76	ASN
1	L	89	GLN
2	H	5	GLN
2	H	77	GLN
3	Y	59	ASN
3	Y	74	ASN
3	Y	77	ASN
3	Y	106	ASN

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 [i](#)

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.