



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:17 PM UTC

PDB ID : 4HYC / pdb_00004hyc
Title : Structure of a presenilin family intramembrane aspartate protease in P2 space group
Authors : Li, X.; Dang, S.; Yan, C.; Wang, J.; Shi, Y.
Deposited on : 2012-11-13
Resolution : 3.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

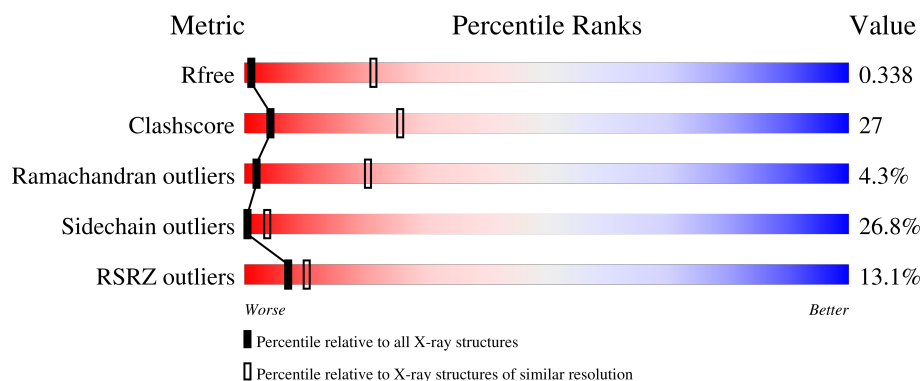
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	
1	E	301	

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Mol	Chain	Length	Quality of chain
1	F	301	12% 32% 36% 13% • 18%
1	G	301	13% 31% 37% 14% 18%
1	H	301	12% 35% 34% 12% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14416 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	B	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	C	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	D	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	E	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	F	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	G	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	H	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			

There are 40 discrepancies between the modelled and reference sequences:

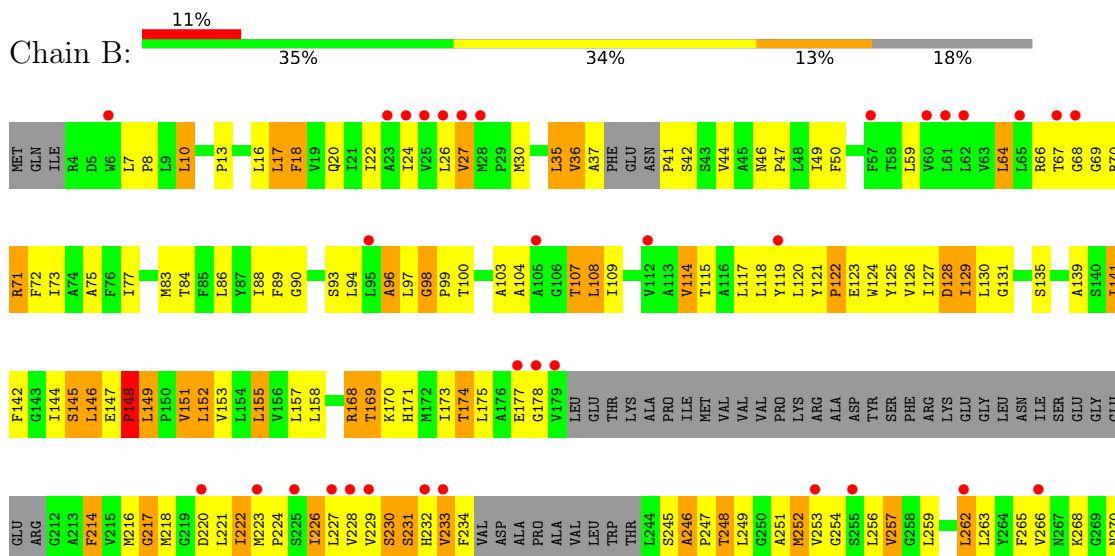
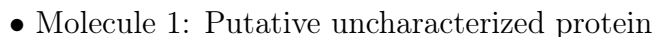
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ASP	engineered mutation	UNP A3CWV0
A	42	SER	GLU	engineered mutation	UNP A3CWV0
A	147	GLU	ALA	engineered mutation	UNP A3CWV0
A	148	PRO	VAL	engineered mutation	UNP A3CWV0
A	229	VAL	ALA	engineered mutation	UNP A3CWV0
B	40	ASN	ASP	engineered mutation	UNP A3CWV0
B	42	SER	GLU	engineered mutation	UNP A3CWV0
B	147	GLU	ALA	engineered mutation	UNP A3CWV0
B	148	PRO	VAL	engineered mutation	UNP A3CWV0
B	229	VAL	ALA	engineered mutation	UNP A3CWV0
C	40	ASN	ASP	engineered mutation	UNP A3CWV0
C	42	SER	GLU	engineered mutation	UNP A3CWV0
C	147	GLU	ALA	engineered mutation	UNP A3CWV0

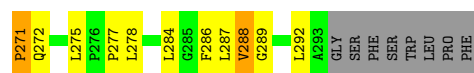
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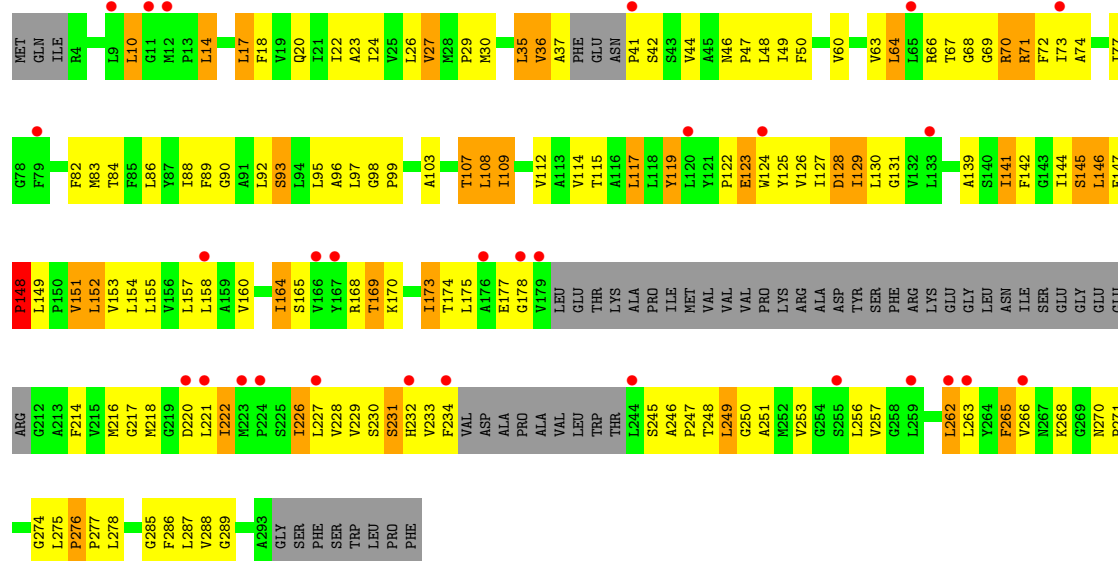
Chain	Residue	Modelled	Actual	Comment	Reference
C	148	PRO	VAL	engineered mutation	UNP A3CWV0
C	229	VAL	ALA	engineered mutation	UNP A3CWV0
D	40	ASN	ASP	engineered mutation	UNP A3CWV0
D	42	SER	GLU	engineered mutation	UNP A3CWV0
D	147	GLU	ALA	engineered mutation	UNP A3CWV0
D	148	PRO	VAL	engineered mutation	UNP A3CWV0
D	229	VAL	ALA	engineered mutation	UNP A3CWV0
E	40	ASN	ASP	engineered mutation	UNP A3CWV0
E	42	SER	GLU	engineered mutation	UNP A3CWV0
E	147	GLU	ALA	engineered mutation	UNP A3CWV0
E	148	PRO	VAL	engineered mutation	UNP A3CWV0
E	229	VAL	ALA	engineered mutation	UNP A3CWV0
F	40	ASN	ASP	engineered mutation	UNP A3CWV0
F	42	SER	GLU	engineered mutation	UNP A3CWV0
F	147	GLU	ALA	engineered mutation	UNP A3CWV0
F	148	PRO	VAL	engineered mutation	UNP A3CWV0
F	229	VAL	ALA	engineered mutation	UNP A3CWV0
G	40	ASN	ASP	engineered mutation	UNP A3CWV0
G	42	SER	GLU	engineered mutation	UNP A3CWV0
G	147	GLU	ALA	engineered mutation	UNP A3CWV0
G	148	PRO	VAL	engineered mutation	UNP A3CWV0
G	229	VAL	ALA	engineered mutation	UNP A3CWV0
H	40	ASN	ASP	engineered mutation	UNP A3CWV0
H	42	SER	GLU	engineered mutation	UNP A3CWV0
H	147	GLU	ALA	engineered mutation	UNP A3CWV0
H	148	PRO	VAL	engineered mutation	UNP A3CWV0
H	229	VAL	ALA	engineered mutation	UNP A3CWV0

- Molecule 1: Putative uncharacterized protein

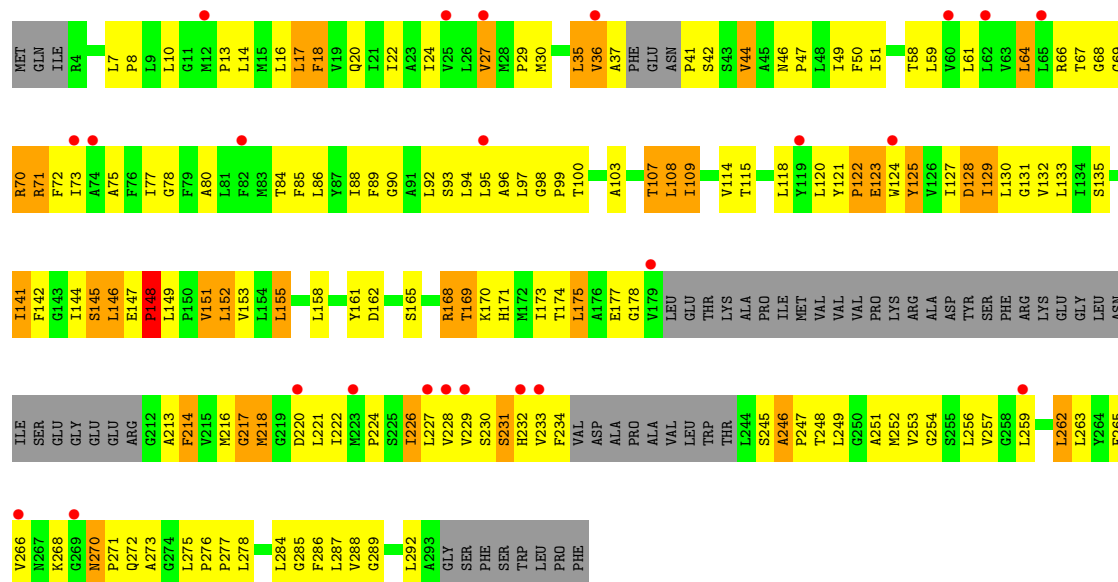




• Molecule 1: Putative uncharacterized protein

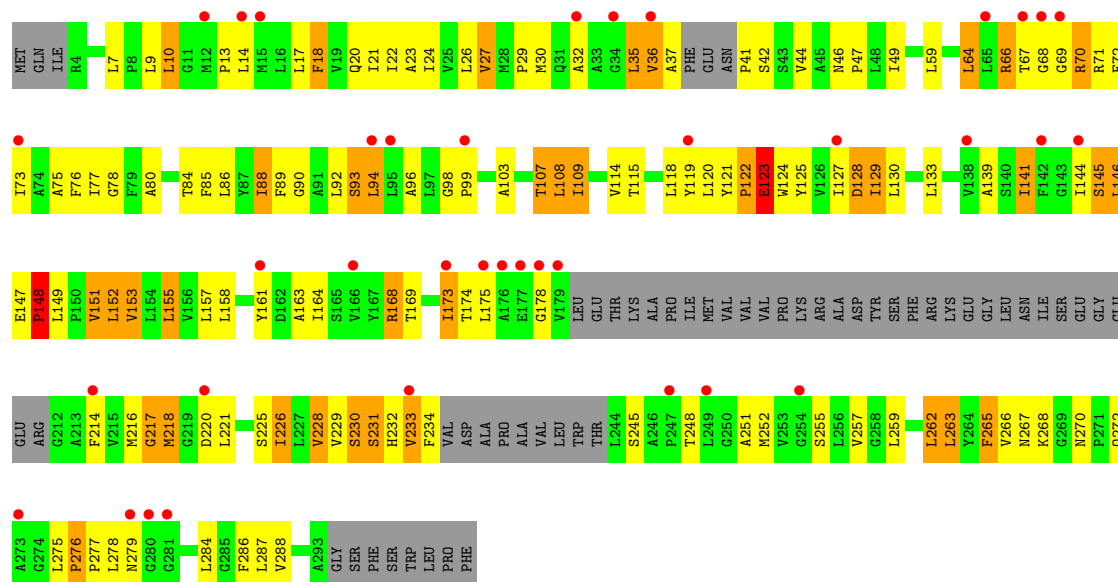


• Molecule 1: Putative uncharacterized protein

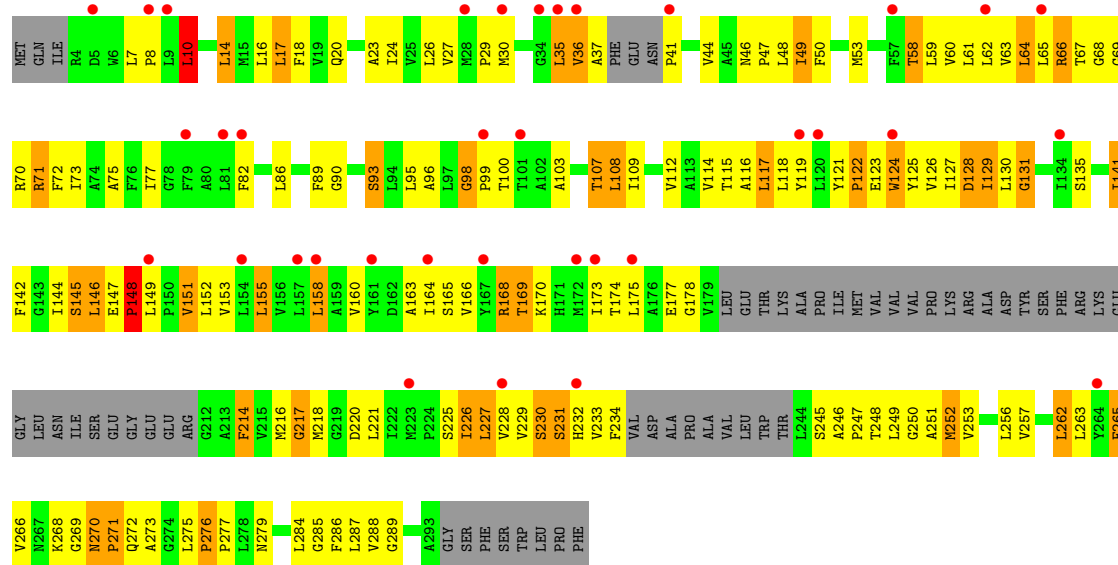


• Molecule 1: Putative uncharacterized protein

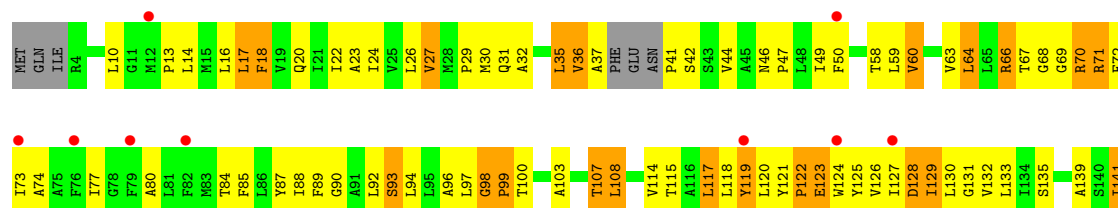


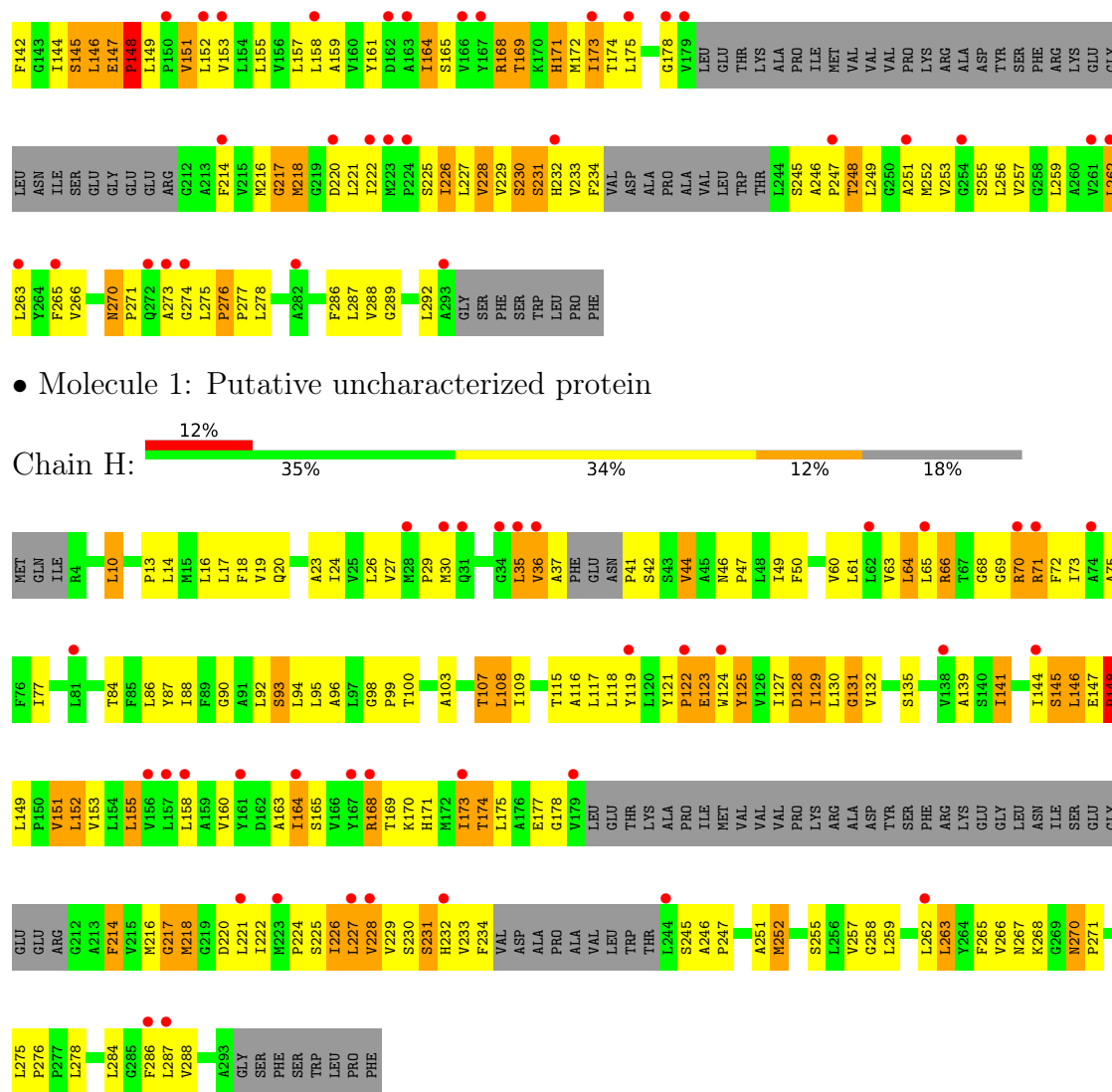


• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein





● Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.22Å 115.83Å 137.17Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	40.16 – 3.95 40.16 – 3.95	Depositor EDS
% Data completeness (in resolution range)	78.3 (40.16-3.95) 78.7 (40.16-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.308 , 0.341 0.309 , 0.338	Depositor DCC
R_{free} test set	1341 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	123.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 94.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14416	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	0.59	0/1839	1.13	13/2511 (0.5%)
1	B	0.61	0/1839	1.12	16/2511 (0.6%)
1	C	0.61	0/1839	1.11	13/2511 (0.5%)
1	D	0.63	0/1839	1.11	12/2511 (0.5%)
1	E	0.63	0/1839	1.14	15/2511 (0.6%)
1	F	0.60	0/1839	1.13	13/2511 (0.5%)
1	G	0.61	0/1839	1.16	18/2511 (0.7%)
1	H	0.58	0/1839	1.06	9/2511 (0.4%)
All	All	0.61	0/14712	1.12	109/20088 (0.5%)

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	2
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	LEU	N-CA-C	10.51	123.34	110.41
1	A	125	TYR	N-CA-C	-10.50	100.21	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	146	LEU	N-CA-C	10.22	122.99	110.41
1	F	270	ASN	CA-C-N	10.05	131.36	120.11
1	F	270	ASN	C-N-CA	10.05	131.36	120.11

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	TRP	Peptide
1	A	145	SER	Peptide
1	B	145	SER	Peptide
1	C	124	TRP	Peptide
1	C	145	SER	Peptide

5.2 Too-close contacts [i](#)

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	1802	0	1949	110	0
1	B	1802	0	1949	102	0
1	C	1802	0	1949	102	0
1	D	1802	0	1949	109	0
1	E	1802	0	1949	104	0
1	F	1802	0	1949	112	0
1	G	1802	0	1949	103	0
1	H	1802	0	1949	108	0
All	All	14416	0	15592	810	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 27.

The worst 5 of 810 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:36:VAL:CG2	1:A:144:ILE:HG22	1.28	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:CG2	1:C:144:ILE:HG22	1.30	1.57
1:F:36:VAL:CG2	1:F:144:ILE:HG22	1.51	1.40
1:A:36:VAL:HG13	1:A:145:SER:CA	1.59	1.32
1:H:36:VAL:CG2	1:H:144:ILE:HG22	1.63	1.29

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	238/301 (79%)	202 (85%)	26 (11%)	10 (4%)	2	20
1	B	238/301 (79%)	196 (82%)	31 (13%)	11 (5%)	2	19
1	C	238/301 (79%)	201 (84%)	27 (11%)	10 (4%)	2	20
1	D	238/301 (79%)	198 (83%)	29 (12%)	11 (5%)	2	19
1	E	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	2	20
1	F	238/301 (79%)	199 (84%)	29 (12%)	10 (4%)	2	20
1	G	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	2	20
1	H	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	2	20
All	All	1904/2408 (79%)	1590 (84%)	232 (12%)	82 (4%)	2	20

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	96	ALA
1	A	230	SER
1	B	36	VAL
1	B	96	ALA

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	A	188/236 (80%)	139 (74%)	49 (26%)	0	4
1	B	188/236 (80%)	140 (74%)	48 (26%)	0	4
1	C	188/236 (80%)	137 (73%)	51 (27%)	0	3
1	D	188/236 (80%)	138 (73%)	50 (27%)	0	4
1	E	188/236 (80%)	139 (74%)	49 (26%)	0	4
1	F	188/236 (80%)	135 (72%)	53 (28%)	0	3
1	G	188/236 (80%)	137 (73%)	51 (27%)	0	3
1	H	188/236 (80%)	136 (72%)	52 (28%)	0	3
All	All	1504/1888 (80%)	1101 (73%)	403 (27%)	0	4

5 of 403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	175	LEU
1	F	227	LEU
1	H	263	LEU
1	E	233	VAL
1	F	107	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	279	ASN
1	G	171	HIS
1	G	267	ASN
1	D	171	HIS
1	B	272	GLN

5.3.3 RNA ⓘ

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	246/301 (81%)	0.64	25 (10%)	12 14	81, 117, 188, 281	0
1	B	246/301 (81%)	0.79	33 (13%)	7 10	92, 120, 194, 266	0
1	C	246/301 (81%)	0.73	29 (11%)	9 12	81, 117, 194, 280	0
1	D	246/301 (81%)	0.75	24 (9%)	13 15	99, 124, 189, 250	0
1	E	246/301 (81%)	0.98	37 (15%)	5 9	86, 137, 203, 289	0
1	F	246/301 (81%)	0.86	35 (14%)	6 9	108, 150, 221, 269	0
1	G	246/301 (81%)	0.88	39 (15%)	5 8	83, 126, 197, 287	0
1	H	246/301 (81%)	0.87	35 (14%)	6 9	142, 173, 247, 299	0
All	All	1968/2408 (81%)	0.81	257 (13%)	7 10	81, 133, 210, 299	0

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	VAL	12.2
1	G	273	ALA	10.7
1	F	232	HIS	10.1
1	H	35	LEU	10.1
1	C	220	ASP	7.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.