



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:18 AM UTC

PDB ID : 8XK5 / pdb_00008xk5
Title : SNB1G11 Fab bound to SFTSV glycoprotein Gn
Authors : Deng, Z.
Deposited on : 2023-12-22
Resolution : 3.05 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

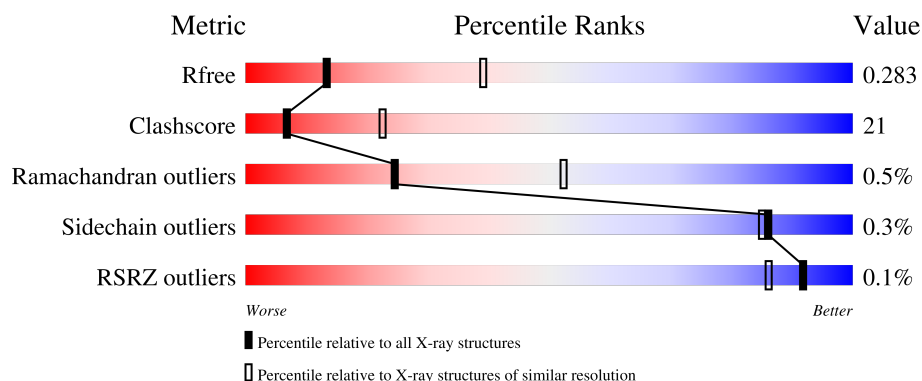
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	256	54% 30% • 14%
1	C	256	50% 34% • 14%
1	G	256	28% 21% 52%
1	I	256	46% 40% 14%
1	N	256	44% 41% • 14%

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Mol	Chain	Length	Quality of chain
2	B	233	
2	D	233	
2	H	233	
2	J	233	
2	O	233	
3	E	357	
3	F	357	
3	K	357	
3	L	357	
3	R	357	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27019 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 mAb SNB1G11 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1686	1070	276	332	8			
1	C	220	Total	C	N	O	S	0	0	0
			1695	1076	278	333	8			
1	I	220	Total	C	N	O	S	0	0	0
			1695	1076	278	333	8			
1	N	219	Total	C	N	O	S	0	0	0
			1689	1073	277	331	8			
1	G	124	Total	C	N	O	S	0	0	0
			997	632	164	195	6			

- Molecule 2 is a protein called mAb SNB1G11 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1620	1016	269	330	5			
2	D	210	Total	C	N	O	S	0	0	0
			1620	1016	269	330	5			
2	J	213	Total	C	N	O	S	0	0	0
			1639	1026	272	335	6			
2	O	212	Total	C	N	O	S	0	0	0
			1633	1023	271	334	5			
2	H	105	Total	C	N	O	S	0	0	0
			804	507	130	164	3			

- Molecule 3 is a protein called Envelopment polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	309	Total	C	N	O	S	0	0	0
			2384	1495	412	451	26			
3	F	309	Total	C	N	O	S	0	0	0
			2384	1495	412	451	26			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	311	Total	C	N	O	S	0	0	0
			2402	1506	415	455	26			
3	R	309	Total	C	N	O	S	0	0	0
			2387	1498	413	450	26			
3	L	309	Total	C	N	O	S	0	0	0
			2384	1495	412	451	26			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	13	LEU	PHE	conflict	UNP R4V2Q5
E	18	GLY	SER	conflict	UNP R4V2Q5
E	21	THR	SER	conflict	UNP R4V2Q5
E	161	ARG	GLY	conflict	UNP R4V2Q5
E	340	SER	ASN	conflict	UNP R4V2Q5
E	341	GLY	-	expression tag	UNP R4V2Q5
E	342	SER	-	expression tag	UNP R4V2Q5
E	343	THR	-	expression tag	UNP R4V2Q5
E	344	LEU	-	expression tag	UNP R4V2Q5
E	345	GLU	-	expression tag	UNP R4V2Q5
E	346	VAL	-	expression tag	UNP R4V2Q5
E	347	LEU	-	expression tag	UNP R4V2Q5
E	348	PHE	-	expression tag	UNP R4V2Q5
E	349	GLN	-	expression tag	UNP R4V2Q5
E	350	GLY	-	expression tag	UNP R4V2Q5
E	351	PRO	-	expression tag	UNP R4V2Q5
E	352	HIS	-	expression tag	UNP R4V2Q5
E	353	HIS	-	expression tag	UNP R4V2Q5
E	354	HIS	-	expression tag	UNP R4V2Q5
E	355	HIS	-	expression tag	UNP R4V2Q5
E	356	HIS	-	expression tag	UNP R4V2Q5
E	357	HIS	-	expression tag	UNP R4V2Q5
F	13	LEU	PHE	conflict	UNP R4V2Q5
F	18	GLY	SER	conflict	UNP R4V2Q5
F	21	THR	SER	conflict	UNP R4V2Q5
F	161	ARG	GLY	conflict	UNP R4V2Q5
F	340	SER	ASN	conflict	UNP R4V2Q5
F	341	GLY	-	expression tag	UNP R4V2Q5
F	342	SER	-	expression tag	UNP R4V2Q5
F	343	THR	-	expression tag	UNP R4V2Q5
F	344	LEU	-	expression tag	UNP R4V2Q5
F	345	GLU	-	expression tag	UNP R4V2Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	346	VAL	-	expression tag	UNP R4V2Q5
F	347	LEU	-	expression tag	UNP R4V2Q5
F	348	PHE	-	expression tag	UNP R4V2Q5
F	349	GLN	-	expression tag	UNP R4V2Q5
F	350	GLY	-	expression tag	UNP R4V2Q5
F	351	PRO	-	expression tag	UNP R4V2Q5
F	352	HIS	-	expression tag	UNP R4V2Q5
F	353	HIS	-	expression tag	UNP R4V2Q5
F	354	HIS	-	expression tag	UNP R4V2Q5
F	355	HIS	-	expression tag	UNP R4V2Q5
F	356	HIS	-	expression tag	UNP R4V2Q5
F	357	HIS	-	expression tag	UNP R4V2Q5
K	13	LEU	PHE	conflict	UNP R4V2Q5
K	18	GLY	SER	conflict	UNP R4V2Q5
K	21	THR	SER	conflict	UNP R4V2Q5
K	161	ARG	GLY	conflict	UNP R4V2Q5
K	340	SER	ASN	conflict	UNP R4V2Q5
K	341	GLY	-	expression tag	UNP R4V2Q5
K	342	SER	-	expression tag	UNP R4V2Q5
K	343	THR	-	expression tag	UNP R4V2Q5
K	344	LEU	-	expression tag	UNP R4V2Q5
K	345	GLU	-	expression tag	UNP R4V2Q5
K	346	VAL	-	expression tag	UNP R4V2Q5
K	347	LEU	-	expression tag	UNP R4V2Q5
K	348	PHE	-	expression tag	UNP R4V2Q5
K	349	GLN	-	expression tag	UNP R4V2Q5
K	350	GLY	-	expression tag	UNP R4V2Q5
K	351	PRO	-	expression tag	UNP R4V2Q5
K	352	HIS	-	expression tag	UNP R4V2Q5
K	353	HIS	-	expression tag	UNP R4V2Q5
K	354	HIS	-	expression tag	UNP R4V2Q5
K	355	HIS	-	expression tag	UNP R4V2Q5
K	356	HIS	-	expression tag	UNP R4V2Q5
K	357	HIS	-	expression tag	UNP R4V2Q5
R	13	LEU	PHE	conflict	UNP R4V2Q5
R	18	GLY	SER	conflict	UNP R4V2Q5
R	21	THR	SER	conflict	UNP R4V2Q5
R	161	ARG	GLY	conflict	UNP R4V2Q5
R	340	SER	ASN	conflict	UNP R4V2Q5
R	341	GLY	-	expression tag	UNP R4V2Q5
R	342	SER	-	expression tag	UNP R4V2Q5
R	343	THR	-	expression tag	UNP R4V2Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	344	LEU	-	expression tag	UNP R4V2Q5
R	345	GLU	-	expression tag	UNP R4V2Q5
R	346	VAL	-	expression tag	UNP R4V2Q5
R	347	LEU	-	expression tag	UNP R4V2Q5
R	348	PHE	-	expression tag	UNP R4V2Q5
R	349	GLN	-	expression tag	UNP R4V2Q5
R	350	GLY	-	expression tag	UNP R4V2Q5
R	351	PRO	-	expression tag	UNP R4V2Q5
R	352	HIS	-	expression tag	UNP R4V2Q5
R	353	HIS	-	expression tag	UNP R4V2Q5
R	354	HIS	-	expression tag	UNP R4V2Q5
R	355	HIS	-	expression tag	UNP R4V2Q5
R	356	HIS	-	expression tag	UNP R4V2Q5
R	357	HIS	-	expression tag	UNP R4V2Q5
L	13	LEU	PHE	conflict	UNP R4V2Q5
L	18	GLY	SER	conflict	UNP R4V2Q5
L	21	THR	SER	conflict	UNP R4V2Q5
L	161	ARG	GLY	conflict	UNP R4V2Q5
L	340	SER	ASN	conflict	UNP R4V2Q5
L	341	GLY	-	expression tag	UNP R4V2Q5
L	342	SER	-	expression tag	UNP R4V2Q5
L	343	THR	-	expression tag	UNP R4V2Q5
L	344	LEU	-	expression tag	UNP R4V2Q5
L	345	GLU	-	expression tag	UNP R4V2Q5
L	346	VAL	-	expression tag	UNP R4V2Q5
L	347	LEU	-	expression tag	UNP R4V2Q5
L	348	PHE	-	expression tag	UNP R4V2Q5
L	349	GLN	-	expression tag	UNP R4V2Q5
L	350	GLY	-	expression tag	UNP R4V2Q5
L	351	PRO	-	expression tag	UNP R4V2Q5
L	352	HIS	-	expression tag	UNP R4V2Q5
L	353	HIS	-	expression tag	UNP R4V2Q5
L	354	HIS	-	expression tag	UNP R4V2Q5
L	355	HIS	-	expression tag	UNP R4V2Q5
L	356	HIS	-	expression tag	UNP R4V2Q5
L	357	HIS	-	expression tag	UNP R4V2Q5

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

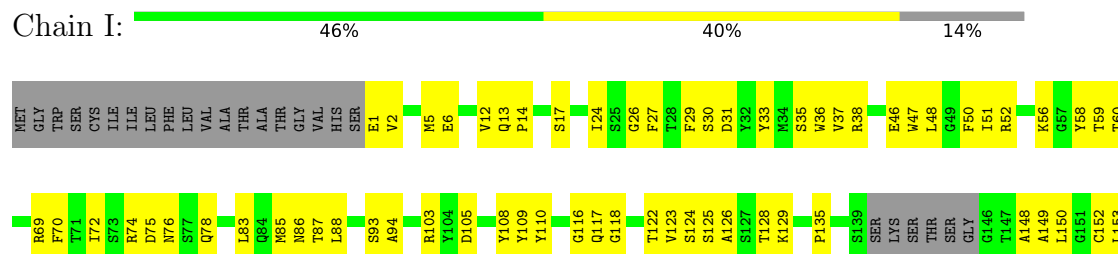
• Molecule 1: mAb SNB1G11 Fab heavy chain



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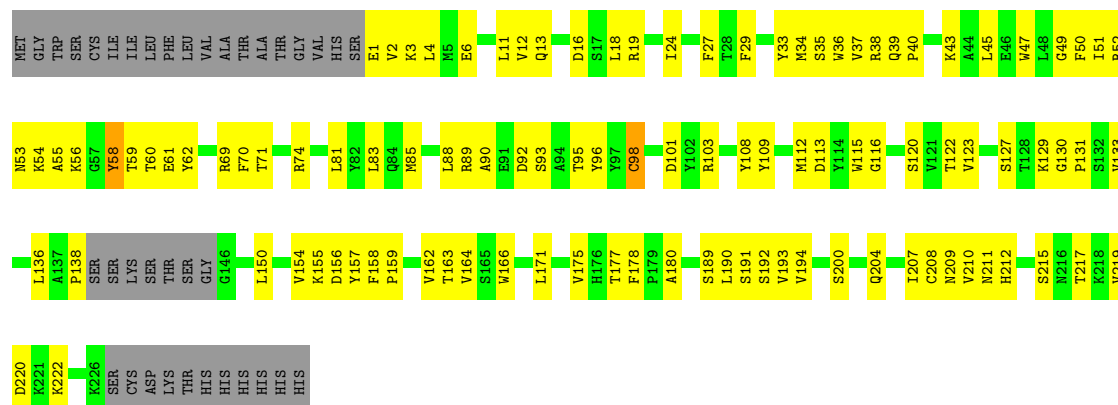


• Molecule 1: mAb SNB1G11 Fab heavy chain

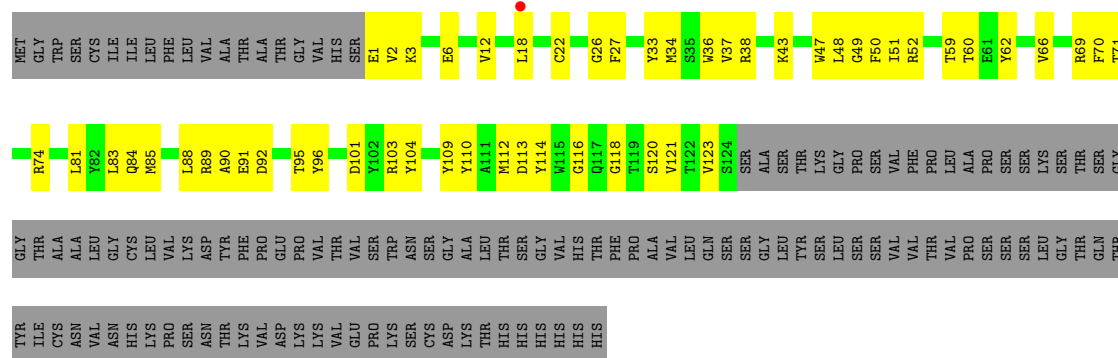
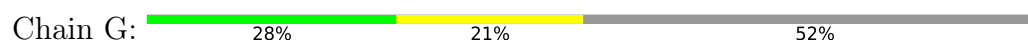




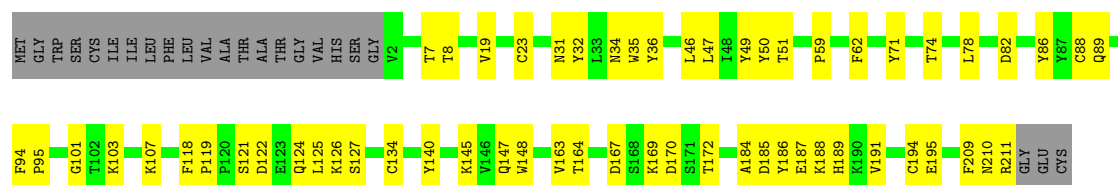
• Molecule 1: mAb SNB1G11 Fab heavy chain



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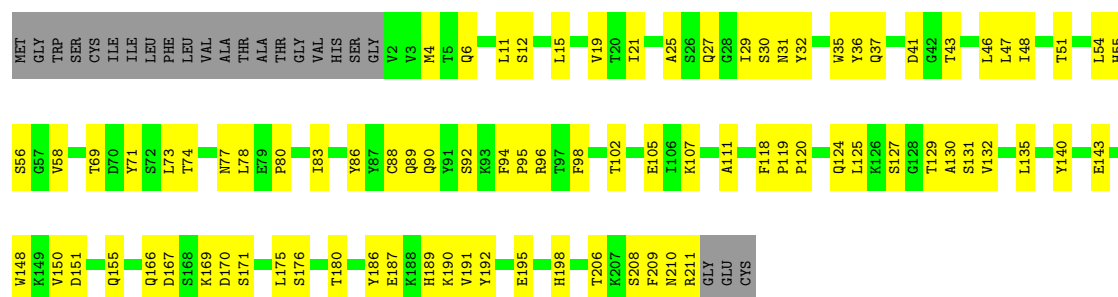


• Molecule 2: mAb SNB1G11 Fab light chain



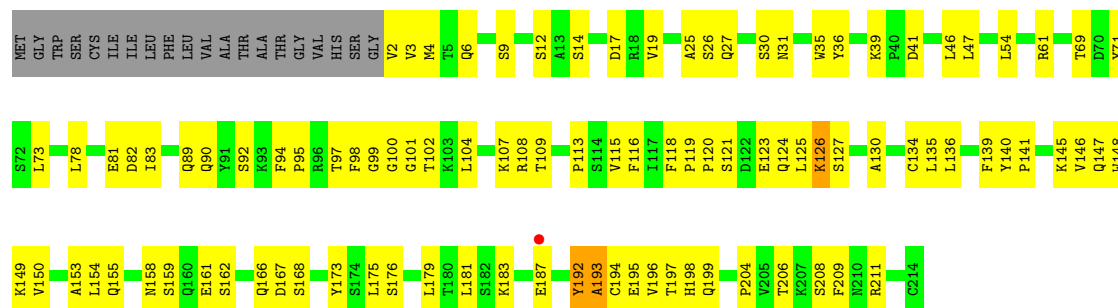
• Molecule 2: mAb SNB1G11 Fab light chain

Chain D: 



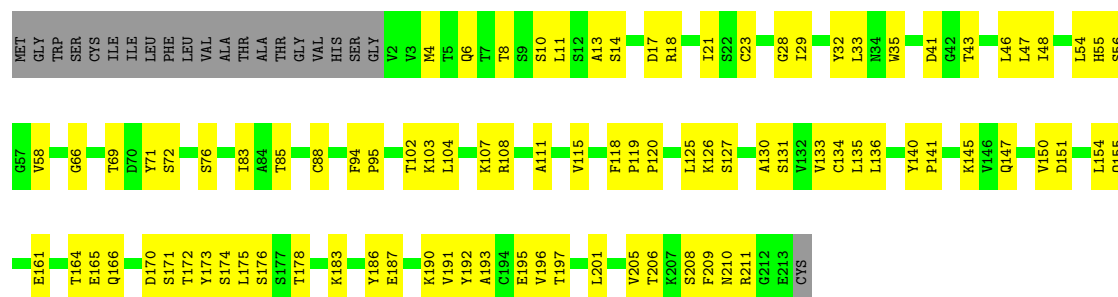
• Molecule 2: mAb SNB1G11 Fab light chain

Chain J: 



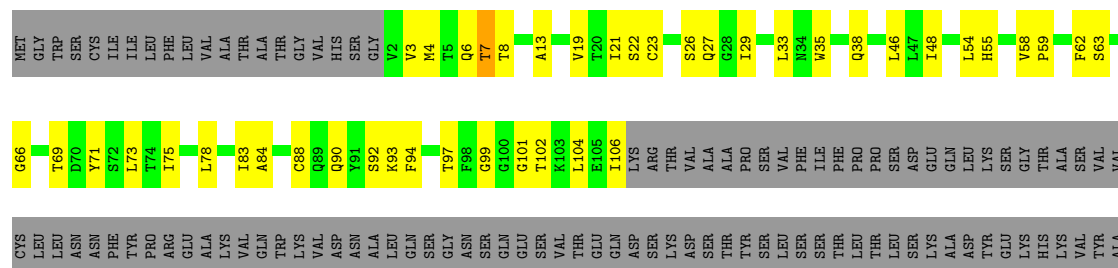
• Molecule 2: mAb SNB1G11 Fab light chain

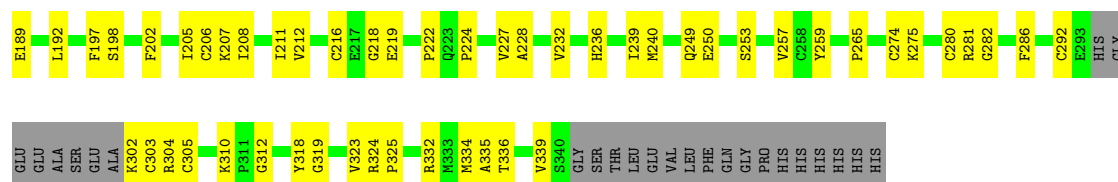
Chain O: 



• Molecule 2: mAb SNB1G11 Fab light chain

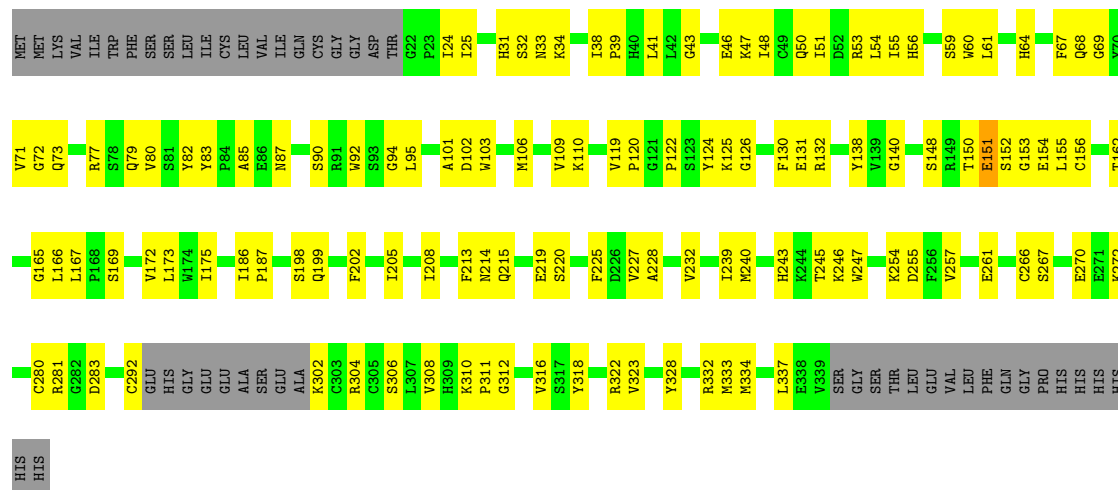
Chain H: 





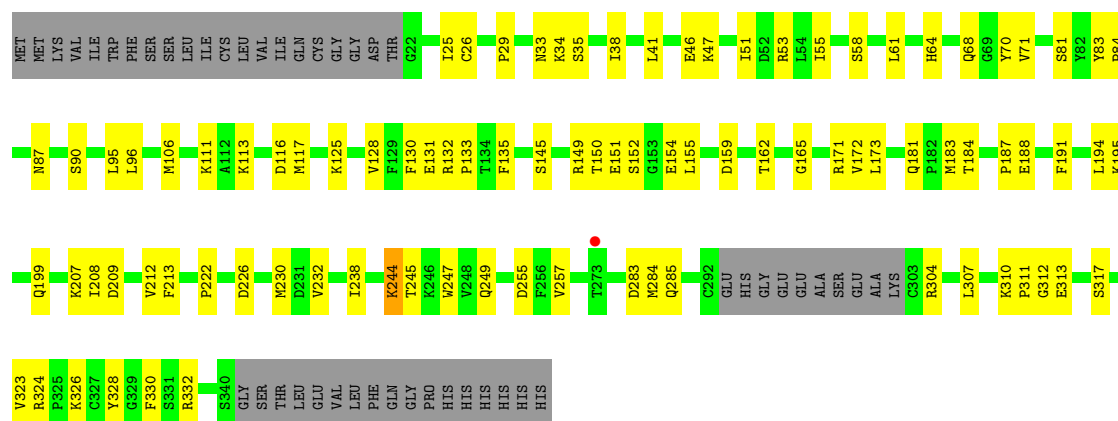
• Molecule 3: Envelopment polypeptide

Chain R: 52% 34% 13%



• Molecule 3: Envelopment polypeptide

Chain L: 61% 25% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.67Å 180.96Å 263.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.05 29.97 – 3.05	Depositor EDS
% Data completeness (in resolution range)	76.4 (29.97-3.05) 99.8 (29.97-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.215 , 0.281 0.233 , 0.283	Depositor DCC
R_{free} test set	5281 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	91.7	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	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	0.94	EDS
Total number of atoms	27019	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 [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	0.70	0/1729	0.99	0/2352
1	C	0.73	0/1738	1.00	2/2363 (0.1%)
1	G	0.33	0/1022	0.57	0/1382
1	I	0.60	1/1738 (0.1%)	0.93	1/2363 (0.0%)
1	N	0.56	0/1732	0.90	2/2355 (0.1%)
2	B	0.65	0/1654	0.91	0/2246
2	D	0.66	0/1654	0.90	2/2246 (0.1%)
2	H	0.30	0/821	0.55	0/1115
2	J	0.52	0/1673	0.85	1/2271 (0.0%)
2	O	0.54	0/1667	0.82	0/2263
3	E	0.49	0/2444	0.78	0/3295
3	F	0.51	0/2444	0.76	0/3295
3	K	0.52	0/2462	0.79	3/3318 (0.1%)
3	L	0.38	0/2444	0.70	1/3295 (0.0%)
3	R	0.47	0/2447	0.79	0/3298
All	All	0.55	1/27669 (0.0%)	0.83	12/37457 (0.0%)

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	A	0	2
1	C	0	1
2	J	0	1
3	R	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	87	THR	CA-CB	-5.29	1.44	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	PRO	CA-N-CD	-7.73	101.17	112.00
1	I	109	TYR	CA-CB-CG	6.01	124.72	113.90
2	D	111	ALA	CA-C-N	-5.67	105.52	122.71
2	D	111	ALA	C-N-CA	-5.67	105.52	122.71
2	J	41	ASP	N-CA-CB	-5.64	100.96	110.49

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PRO	Peptide
1	A	146	PHE	Peptide
1	C	158	PHE	Peptide
2	J	192	TYR	Peptide
3	R	151	GLU	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	1686	0	1628	71	0
1	C	1695	0	1641	74	0
1	G	997	0	941	49	0
1	I	1695	0	1641	109	0
1	N	1689	0	1636	102	0
2	B	1620	0	1577	47	0
2	D	1620	0	1577	69	0
2	H	804	0	779	32	0
2	J	1639	0	1593	101	0
2	O	1633	0	1586	84	0
3	E	2384	0	2295	118	0
3	F	2384	0	2295	84	0
3	K	2402	0	2314	81	0
3	L	2384	0	2295	57	0
3	R	2387	0	2303	104	0
All	All	27019	0	26101	1139	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 21.

The worst 5 of 1139 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:I:218:LYS:HG2	1:N:13:GLN:NE2	1.45	1.28
3:E:217:GLU:HG2	3:E:218:GLY:H	1.20	1.06
3:E:201:GLU:O	3:E:241:ARG:NH2	1.92	1.00
1:A:52:ARG:NH2	1:A:58:GLU:OE2	1.95	0.98
1:I:14:PRO:HD2	1:I:125:SER:HB2	1.47	0.95

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	A	215/256 (84%)	198 (92%)	14 (6%)	3 (1%)	9	29
1	C	216/256 (84%)	202 (94%)	11 (5%)	3 (1%)	9	29
1	G	122/256 (48%)	116 (95%)	6 (5%)	0	100	100
1	I	216/256 (84%)	200 (93%)	13 (6%)	3 (1%)	9	29
1	N	215/256 (84%)	200 (93%)	14 (6%)	1 (0%)	24	52
2	B	208/233 (89%)	201 (97%)	7 (3%)	0	100	100
2	D	208/233 (89%)	195 (94%)	13 (6%)	0	100	100
2	H	103/233 (44%)	93 (90%)	9 (9%)	1 (1%)	12	37
2	J	211/233 (91%)	193 (92%)	16 (8%)	2 (1%)	14	39
2	O	210/233 (90%)	198 (94%)	11 (5%)	1 (0%)	24	52
3	E	305/357 (85%)	292 (96%)	11 (4%)	2 (1%)	18	45
3	F	305/357 (85%)	288 (94%)	16 (5%)	1 (0%)	36	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	307/357 (86%)	293 (95%)	14 (5%)	0	100	100
3	L	305/357 (85%)	293 (96%)	12 (4%)	0	100	100
3	R	305/357 (85%)	291 (95%)	14 (5%)	0	100	100
All	All	3451/4230 (82%)	3253 (94%)	181 (5%)	17 (0%)	24	52

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	147	PRO
1	C	105	ASP
1	C	159	PRO
1	I	160	GLU

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	187/219 (85%)	187 (100%)	0	100	100
1	C	188/219 (86%)	187 (100%)	1 (0%)	81	82
1	G	105/219 (48%)	105 (100%)	0	100	100
1	I	188/219 (86%)	187 (100%)	1 (0%)	81	82
1	N	187/219 (85%)	186 (100%)	1 (0%)	81	82
2	B	187/204 (92%)	187 (100%)	0	100	100
2	D	187/204 (92%)	187 (100%)	0	100	100
2	H	92/204 (45%)	92 (100%)	0	100	100
2	J	189/204 (93%)	189 (100%)	0	100	100
2	O	188/204 (92%)	187 (100%)	1 (0%)	81	82
3	E	268/309 (87%)	267 (100%)	1 (0%)	84	84
3	F	268/309 (87%)	266 (99%)	2 (1%)	76	80
3	K	270/309 (87%)	269 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	268/309 (87%)	268 (100%)	0	100	100
3	R	268/309 (87%)	268 (100%)	0	100	100
All	All	3040/3660 (83%)	3032 (100%)	8 (0%)	86	85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	134	CYS
1	N	98	CYS
1	I	152	CYS
3	F	305	CYS
3	K	274	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	53	ASN
3	R	73	GLN
2	H	38	GLN
3	R	50	GLN
3	R	199	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 [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	219/256 (85%)	-0.89	0 100 100	5, 16, 39, 47	0
1	C	220/256 (85%)	-0.88	0 100 100	5, 16, 53, 70	0
1	G	124/256 (48%)	-0.51	1 (0%) 82 63	75, 93, 114, 127	0
1	I	220/256 (85%)	-0.71	0 100 100	11, 33, 97, 106	0
1	N	219/256 (85%)	-0.69	0 100 100	9, 38, 74, 86	0
2	B	210/233 (90%)	-0.89	0 100 100	6, 21, 58, 76	0
2	D	210/233 (90%)	-0.83	0 100 100	5, 18, 58, 64	0
2	H	105/233 (45%)	-0.38	0 100 100	85, 110, 129, 137	0
2	J	213/233 (91%)	-0.51	1 (0%) 87 72	8, 49, 105, 116	0
2	O	212/233 (90%)	-0.74	0 100 100	10, 42, 78, 105	0
3	E	309/357 (86%)	-0.69	0 100 100	10, 56, 83, 101	0
3	F	309/357 (86%)	-0.78	1 (0%) 90 80	11, 39, 80, 93	0
3	K	311/357 (87%)	-0.86	0 100 100	14, 33, 67, 85	0
3	L	309/357 (86%)	-0.48	1 (0%) 90 80	56, 81, 117, 143	0
3	R	309/357 (86%)	-0.82	0 100 100	16, 44, 73, 99	0
All	All	3499/4230 (82%)	-0.73	4 (0%) 92 86	5, 40, 103, 143	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	289	VAL	3.2
1	G	18	LEU	2.9
2	J	187	GLU	2.5
3	L	273	THR	2.2

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.