



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 AM UTC

PDB ID : 3EQ5 / pdb_00003eq5
Title : Crystal structure of fragment 137 to 238 of the human Ski-like protein
Authors : Tresaugues, L.; Wisniewska, M.; Andersson, J.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Moche, M.; Nilsson, M.E.; Nyman, T.; Olesen, K.; Persson, C.; Sagemark, J.; Schueler, H.; Thorsell, A.G.; Van Den Berg, S.; Welin, M.; Wikstrom, M.; Weigelt, J.; Nordlund, P.; Structural Genomics Consortium (SGC)
Deposited on : 2008-09-30
Resolution : 2.45 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)	:	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)

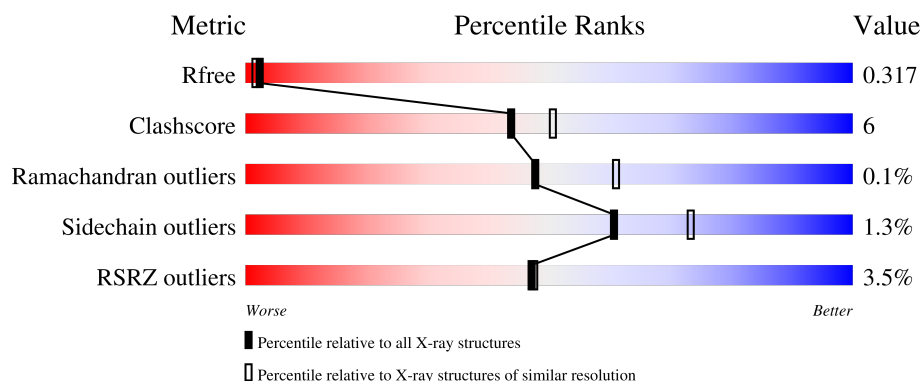
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

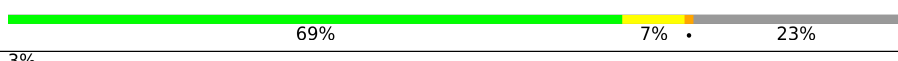
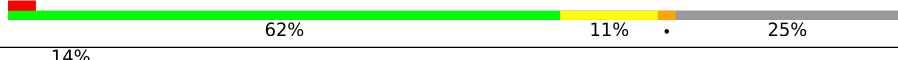
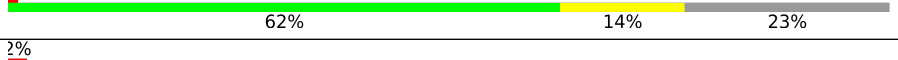
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	125	
1	B	125	
1	C	125	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	125	
1	E	125	
1	F	125	
1	G	125	
1	H	125	
1	I	125	
1	J	125	
1	K	125	
1	L	125	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9437 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 Ski-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	3	0
			796	498	133	155	10			
1	B	97	Total	C	N	O	S	0	5	0
			782	497	132	146	7			
1	C	97	Total	C	N	O	S	0	1	0
			761	478	133	143	7			
1	D	96	Total	C	N	O	S	0	1	0
			748	471	126	144	7			
1	E	95	Total	C	N	O	S	0	1	0
			747	470	129	141	7			
1	F	98	Total	C	N	O	S	0	2	0
			781	488	137	149	7			
1	G	95	Total	C	N	O	S	0	0	0
			735	462	125	141	7			
1	H	96	Total	C	N	O	S	0	2	0
			754	475	129	143	7			
1	I	94	Total	C	N	O	S	0	3	0
			750	473	132	138	7			
1	J	96	Total	C	N	O	S	0	1	0
			751	472	129	142	8			
1	K	96	Total	C	N	O	S	0	1	0
			752	473	129	143	7			
1	L	94	Total	C	N	O	S	0	1	0
			737	464	128	138	7			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	MET	-	expression tag	UNP P12757
A	115	HIS	-	expression tag	UNP P12757
A	116	HIS	-	expression tag	UNP P12757
A	117	HIS	-	expression tag	UNP P12757
A	118	HIS	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
A	119	HIS	-	expression tag	UNP P12757
A	120	HIS	-	expression tag	UNP P12757
A	121	SER	-	expression tag	UNP P12757
A	122	SER	-	expression tag	UNP P12757
A	123	GLY	-	expression tag	UNP P12757
A	124	VAL	-	expression tag	UNP P12757
A	125	ASP	-	expression tag	UNP P12757
A	126	LEU	-	expression tag	UNP P12757
A	127	GLY	-	expression tag	UNP P12757
A	128	THR	-	expression tag	UNP P12757
A	129	GLU	-	expression tag	UNP P12757
A	130	ASN	-	expression tag	UNP P12757
A	131	LEU	-	expression tag	UNP P12757
A	132	TYR	-	expression tag	UNP P12757
A	133	PHE	-	expression tag	UNP P12757
A	134	GLN	-	expression tag	UNP P12757
A	135	SER	-	expression tag	UNP P12757
A	136	MET	-	expression tag	UNP P12757
B	114	MET	-	expression tag	UNP P12757
B	115	HIS	-	expression tag	UNP P12757
B	116	HIS	-	expression tag	UNP P12757
B	117	HIS	-	expression tag	UNP P12757
B	118	HIS	-	expression tag	UNP P12757
B	119	HIS	-	expression tag	UNP P12757
B	120	HIS	-	expression tag	UNP P12757
B	121	SER	-	expression tag	UNP P12757
B	122	SER	-	expression tag	UNP P12757
B	123	GLY	-	expression tag	UNP P12757
B	124	VAL	-	expression tag	UNP P12757
B	125	ASP	-	expression tag	UNP P12757
B	126	LEU	-	expression tag	UNP P12757
B	127	GLY	-	expression tag	UNP P12757
B	128	THR	-	expression tag	UNP P12757
B	129	GLU	-	expression tag	UNP P12757
B	130	ASN	-	expression tag	UNP P12757
B	131	LEU	-	expression tag	UNP P12757
B	132	TYR	-	expression tag	UNP P12757
B	133	PHE	-	expression tag	UNP P12757
B	134	GLN	-	expression tag	UNP P12757
B	135	SER	-	expression tag	UNP P12757
B	136	MET	-	expression tag	UNP P12757
C	114	MET	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
C	115	HIS	-	expression tag	UNP P12757
C	116	HIS	-	expression tag	UNP P12757
C	117	HIS	-	expression tag	UNP P12757
C	118	HIS	-	expression tag	UNP P12757
C	119	HIS	-	expression tag	UNP P12757
C	120	HIS	-	expression tag	UNP P12757
C	121	SER	-	expression tag	UNP P12757
C	122	SER	-	expression tag	UNP P12757
C	123	GLY	-	expression tag	UNP P12757
C	124	VAL	-	expression tag	UNP P12757
C	125	ASP	-	expression tag	UNP P12757
C	126	LEU	-	expression tag	UNP P12757
C	127	GLY	-	expression tag	UNP P12757
C	128	THR	-	expression tag	UNP P12757
C	129	GLU	-	expression tag	UNP P12757
C	130	ASN	-	expression tag	UNP P12757
C	131	LEU	-	expression tag	UNP P12757
C	132	TYR	-	expression tag	UNP P12757
C	133	PHE	-	expression tag	UNP P12757
C	134	GLN	-	expression tag	UNP P12757
C	135	SER	-	expression tag	UNP P12757
C	136	MET	-	expression tag	UNP P12757
D	114	MET	-	expression tag	UNP P12757
D	115	HIS	-	expression tag	UNP P12757
D	116	HIS	-	expression tag	UNP P12757
D	117	HIS	-	expression tag	UNP P12757
D	118	HIS	-	expression tag	UNP P12757
D	119	HIS	-	expression tag	UNP P12757
D	120	HIS	-	expression tag	UNP P12757
D	121	SER	-	expression tag	UNP P12757
D	122	SER	-	expression tag	UNP P12757
D	123	GLY	-	expression tag	UNP P12757
D	124	VAL	-	expression tag	UNP P12757
D	125	ASP	-	expression tag	UNP P12757
D	126	LEU	-	expression tag	UNP P12757
D	127	GLY	-	expression tag	UNP P12757
D	128	THR	-	expression tag	UNP P12757
D	129	GLU	-	expression tag	UNP P12757
D	130	ASN	-	expression tag	UNP P12757
D	131	LEU	-	expression tag	UNP P12757
D	132	TYR	-	expression tag	UNP P12757
D	133	PHE	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
D	134	GLN	-	expression tag	UNP P12757
D	135	SER	-	expression tag	UNP P12757
D	136	MET	-	expression tag	UNP P12757
E	114	MET	-	expression tag	UNP P12757
E	115	HIS	-	expression tag	UNP P12757
E	116	HIS	-	expression tag	UNP P12757
E	117	HIS	-	expression tag	UNP P12757
E	118	HIS	-	expression tag	UNP P12757
E	119	HIS	-	expression tag	UNP P12757
E	120	HIS	-	expression tag	UNP P12757
E	121	SER	-	expression tag	UNP P12757
E	122	SER	-	expression tag	UNP P12757
E	123	GLY	-	expression tag	UNP P12757
E	124	VAL	-	expression tag	UNP P12757
E	125	ASP	-	expression tag	UNP P12757
E	126	LEU	-	expression tag	UNP P12757
E	127	GLY	-	expression tag	UNP P12757
E	128	THR	-	expression tag	UNP P12757
E	129	GLU	-	expression tag	UNP P12757
E	130	ASN	-	expression tag	UNP P12757
E	131	LEU	-	expression tag	UNP P12757
E	132	TYR	-	expression tag	UNP P12757
E	133	PHE	-	expression tag	UNP P12757
E	134	GLN	-	expression tag	UNP P12757
E	135	SER	-	expression tag	UNP P12757
E	136	MET	-	expression tag	UNP P12757
F	114	MET	-	expression tag	UNP P12757
F	115	HIS	-	expression tag	UNP P12757
F	116	HIS	-	expression tag	UNP P12757
F	117	HIS	-	expression tag	UNP P12757
F	118	HIS	-	expression tag	UNP P12757
F	119	HIS	-	expression tag	UNP P12757
F	120	HIS	-	expression tag	UNP P12757
F	121	SER	-	expression tag	UNP P12757
F	122	SER	-	expression tag	UNP P12757
F	123	GLY	-	expression tag	UNP P12757
F	124	VAL	-	expression tag	UNP P12757
F	125	ASP	-	expression tag	UNP P12757
F	126	LEU	-	expression tag	UNP P12757
F	127	GLY	-	expression tag	UNP P12757
F	128	THR	-	expression tag	UNP P12757
F	129	GLU	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
F	130	ASN	-	expression tag	UNP P12757
F	131	LEU	-	expression tag	UNP P12757
F	132	TYR	-	expression tag	UNP P12757
F	133	PHE	-	expression tag	UNP P12757
F	134	GLN	-	expression tag	UNP P12757
F	135	SER	-	expression tag	UNP P12757
F	136	MET	-	expression tag	UNP P12757
G	114	MET	-	expression tag	UNP P12757
G	115	HIS	-	expression tag	UNP P12757
G	116	HIS	-	expression tag	UNP P12757
G	117	HIS	-	expression tag	UNP P12757
G	118	HIS	-	expression tag	UNP P12757
G	119	HIS	-	expression tag	UNP P12757
G	120	HIS	-	expression tag	UNP P12757
G	121	SER	-	expression tag	UNP P12757
G	122	SER	-	expression tag	UNP P12757
G	123	GLY	-	expression tag	UNP P12757
G	124	VAL	-	expression tag	UNP P12757
G	125	ASP	-	expression tag	UNP P12757
G	126	LEU	-	expression tag	UNP P12757
G	127	GLY	-	expression tag	UNP P12757
G	128	THR	-	expression tag	UNP P12757
G	129	GLU	-	expression tag	UNP P12757
G	130	ASN	-	expression tag	UNP P12757
G	131	LEU	-	expression tag	UNP P12757
G	132	TYR	-	expression tag	UNP P12757
G	133	PHE	-	expression tag	UNP P12757
G	134	GLN	-	expression tag	UNP P12757
G	135	SER	-	expression tag	UNP P12757
G	136	MET	-	expression tag	UNP P12757
H	114	MET	-	expression tag	UNP P12757
H	115	HIS	-	expression tag	UNP P12757
H	116	HIS	-	expression tag	UNP P12757
H	117	HIS	-	expression tag	UNP P12757
H	118	HIS	-	expression tag	UNP P12757
H	119	HIS	-	expression tag	UNP P12757
H	120	HIS	-	expression tag	UNP P12757
H	121	SER	-	expression tag	UNP P12757
H	122	SER	-	expression tag	UNP P12757
H	123	GLY	-	expression tag	UNP P12757
H	124	VAL	-	expression tag	UNP P12757
H	125	ASP	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
H	126	LEU	-	expression tag	UNP P12757
H	127	GLY	-	expression tag	UNP P12757
H	128	THR	-	expression tag	UNP P12757
H	129	GLU	-	expression tag	UNP P12757
H	130	ASN	-	expression tag	UNP P12757
H	131	LEU	-	expression tag	UNP P12757
H	132	TYR	-	expression tag	UNP P12757
H	133	PHE	-	expression tag	UNP P12757
H	134	GLN	-	expression tag	UNP P12757
H	135	SER	-	expression tag	UNP P12757
H	136	MET	-	expression tag	UNP P12757
I	114	MET	-	expression tag	UNP P12757
I	115	HIS	-	expression tag	UNP P12757
I	116	HIS	-	expression tag	UNP P12757
I	117	HIS	-	expression tag	UNP P12757
I	118	HIS	-	expression tag	UNP P12757
I	119	HIS	-	expression tag	UNP P12757
I	120	HIS	-	expression tag	UNP P12757
I	121	SER	-	expression tag	UNP P12757
I	122	SER	-	expression tag	UNP P12757
I	123	GLY	-	expression tag	UNP P12757
I	124	VAL	-	expression tag	UNP P12757
I	125	ASP	-	expression tag	UNP P12757
I	126	LEU	-	expression tag	UNP P12757
I	127	GLY	-	expression tag	UNP P12757
I	128	THR	-	expression tag	UNP P12757
I	129	GLU	-	expression tag	UNP P12757
I	130	ASN	-	expression tag	UNP P12757
I	131	LEU	-	expression tag	UNP P12757
I	132	TYR	-	expression tag	UNP P12757
I	133	PHE	-	expression tag	UNP P12757
I	134	GLN	-	expression tag	UNP P12757
I	135	SER	-	expression tag	UNP P12757
I	136	MET	-	expression tag	UNP P12757
J	114	MET	-	expression tag	UNP P12757
J	115	HIS	-	expression tag	UNP P12757
J	116	HIS	-	expression tag	UNP P12757
J	117	HIS	-	expression tag	UNP P12757
J	118	HIS	-	expression tag	UNP P12757
J	119	HIS	-	expression tag	UNP P12757
J	120	HIS	-	expression tag	UNP P12757
J	121	SER	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
J	122	SER	-	expression tag	UNP P12757
J	123	GLY	-	expression tag	UNP P12757
J	124	VAL	-	expression tag	UNP P12757
J	125	ASP	-	expression tag	UNP P12757
J	126	LEU	-	expression tag	UNP P12757
J	127	GLY	-	expression tag	UNP P12757
J	128	THR	-	expression tag	UNP P12757
J	129	GLU	-	expression tag	UNP P12757
J	130	ASN	-	expression tag	UNP P12757
J	131	LEU	-	expression tag	UNP P12757
J	132	TYR	-	expression tag	UNP P12757
J	133	PHE	-	expression tag	UNP P12757
J	134	GLN	-	expression tag	UNP P12757
J	135	SER	-	expression tag	UNP P12757
J	136	MET	-	expression tag	UNP P12757
K	114	MET	-	expression tag	UNP P12757
K	115	HIS	-	expression tag	UNP P12757
K	116	HIS	-	expression tag	UNP P12757
K	117	HIS	-	expression tag	UNP P12757
K	118	HIS	-	expression tag	UNP P12757
K	119	HIS	-	expression tag	UNP P12757
K	120	HIS	-	expression tag	UNP P12757
K	121	SER	-	expression tag	UNP P12757
K	122	SER	-	expression tag	UNP P12757
K	123	GLY	-	expression tag	UNP P12757
K	124	VAL	-	expression tag	UNP P12757
K	125	ASP	-	expression tag	UNP P12757
K	126	LEU	-	expression tag	UNP P12757
K	127	GLY	-	expression tag	UNP P12757
K	128	THR	-	expression tag	UNP P12757
K	129	GLU	-	expression tag	UNP P12757
K	130	ASN	-	expression tag	UNP P12757
K	131	LEU	-	expression tag	UNP P12757
K	132	TYR	-	expression tag	UNP P12757
K	133	PHE	-	expression tag	UNP P12757
K	134	GLN	-	expression tag	UNP P12757
K	135	SER	-	expression tag	UNP P12757
K	136	MET	-	expression tag	UNP P12757
L	114	MET	-	expression tag	UNP P12757
L	115	HIS	-	expression tag	UNP P12757
L	116	HIS	-	expression tag	UNP P12757
L	117	HIS	-	expression tag	UNP P12757

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Chain	Residue	Modelled	Actual	Comment	Reference
L	118	HIS	-	expression tag	UNP P12757
L	119	HIS	-	expression tag	UNP P12757
L	120	HIS	-	expression tag	UNP P12757
L	121	SER	-	expression tag	UNP P12757
L	122	SER	-	expression tag	UNP P12757
L	123	GLY	-	expression tag	UNP P12757
L	124	VAL	-	expression tag	UNP P12757
L	125	ASP	-	expression tag	UNP P12757
L	126	LEU	-	expression tag	UNP P12757
L	127	GLY	-	expression tag	UNP P12757
L	128	THR	-	expression tag	UNP P12757
L	129	GLU	-	expression tag	UNP P12757
L	130	ASN	-	expression tag	UNP P12757
L	131	LEU	-	expression tag	UNP P12757
L	132	TYR	-	expression tag	UNP P12757
L	133	PHE	-	expression tag	UNP P12757
L	134	GLN	-	expression tag	UNP P12757
L	135	SER	-	expression tag	UNP P12757
L	136	MET	-	expression tag	UNP P12757

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	61	Total O 61 61	0	0
2	B	47	Total O 47 47	0	0
2	C	30	Total O 30 30	0	0
2	D	23	Total O 23 23	0	0
2	E	9	Total O 9 9	0	0
2	F	32	Total O 32 32	0	0
2	G	10	Total O 10 10	0	0
2	H	20	Total O 20 20	0	0
2	I	36	Total O 36 36	0	0
2	J	43	Total O 43 43	0	0

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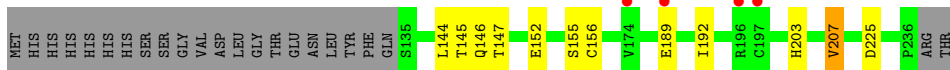
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	16	Total	O	0	0
			16	16		
2	L	16	Total	O	0	0
			16	16		

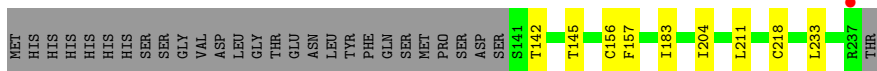
3 Residue-property plots [i](#)

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.

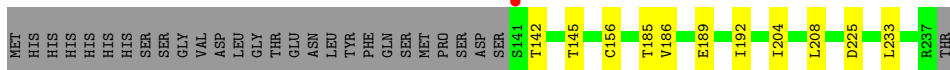
- Molecule 1: Ski-like protein



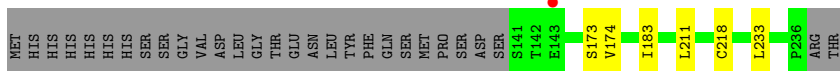
- Molecule 1: Ski-like protein



- Molecule 1: Ski-like protein



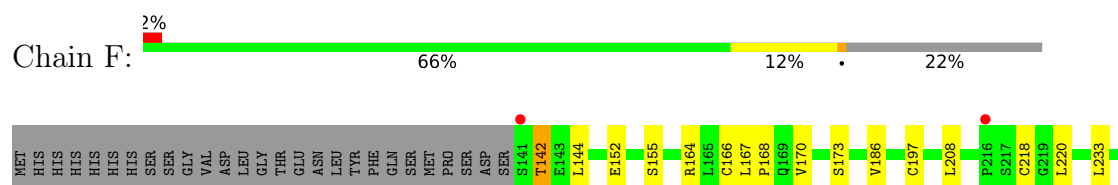
- Molecule 1: Ski-like protein



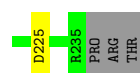
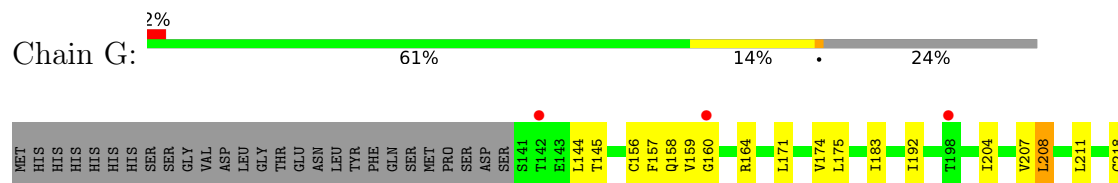
- Molecule 1: Ski-like protein



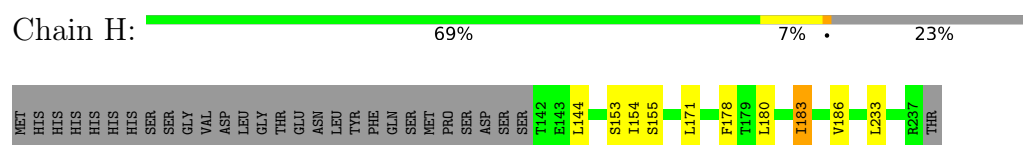
- Molecule 1: Ski-like protein



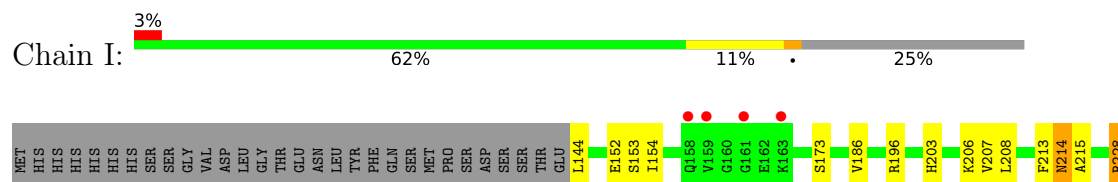
- Molecule 1: Ski-like protein



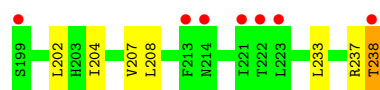
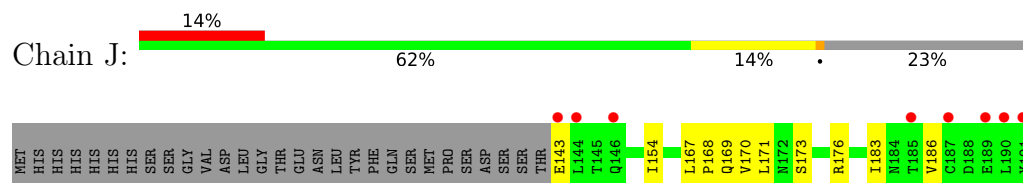
- Molecule 1: Ski-like protein



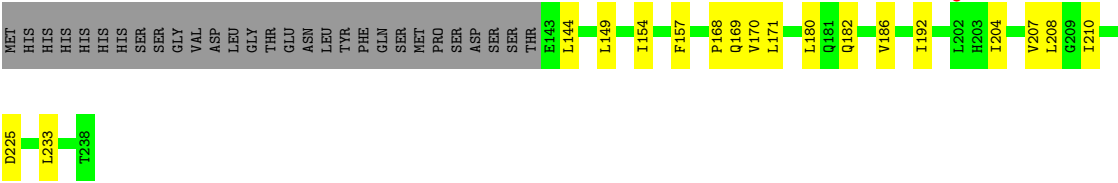
- Molecule 1: Ski-like protein



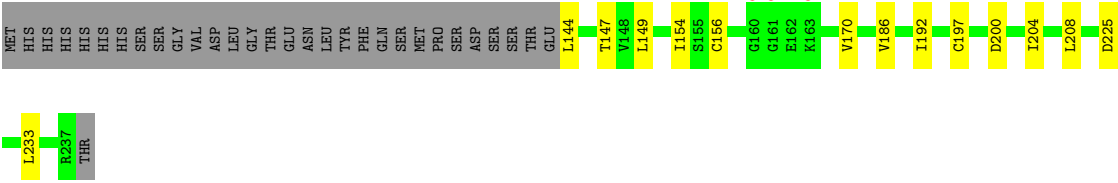
- Molecule 1: Ski-like protein



- Molecule 1: Ski-like protein



● Molecule 1: Ski-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.82Å 70.12Å 116.28Å 90.00° 100.95° 90.00°	Depositor
Resolution (Å)	19.83 – 2.45 19.83 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.83-2.45) 97.8 (19.83-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.232 , 0.274 0.277 , 0.317	Depositor DCC
R_{free} test set	3018 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9437	wwPDB-VP
Average B, all atoms (Å ²)	3.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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	0.47	0/812	0.67	0/1103
1	B	0.42	0/807	0.68	0/1094
1	C	0.41	0/772	0.66	0/1045
1	D	0.43	0/760	0.67	0/1032
1	E	0.43	0/756	0.68	0/1026
1	F	0.43	0/790	0.70	0/1070
1	G	0.45	0/743	0.68	0/1008
1	H	0.41	0/769	0.66	0/1044
1	I	0.45	0/768	0.69	0/1041
1	J	0.44	0/763	0.70	0/1034
1	K	0.41	0/764	0.66	0/1036
1	L	0.43	0/746	0.68	0/1012
All	All	0.43	0/9250	0.68	0/12545

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	796	0	812	5	0
1	B	782	0	820	7	0
1	C	761	0	787	6	0
1	D	748	0	767	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	747	0	768	8	0
1	F	781	0	800	9	0
1	G	735	0	754	13	0
1	H	754	0	781	6	0
1	I	750	0	783	17	0
1	J	751	0	774	13	0
1	K	752	0	776	14	0
1	L	737	0	760	11	0
2	A	61	0	0	0	0
2	B	47	0	0	1	0
2	C	30	0	0	0	0
2	D	23	0	0	0	0
2	E	9	0	0	2	0
2	F	32	0	0	0	0
2	G	10	0	0	0	0
2	H	20	0	0	0	0
2	I	36	0	0	1	0
2	J	43	0	0	0	0
2	K	16	0	0	0	0
2	L	16	0	0	0	0
All	All	9437	0	9382	113	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 6.

All (113) 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:228[A]:ARG:HH11	1:I:228[A]:ARG:CG	1.70	1.05
1:I:228[A]:ARG:HG3	1:I:228[A]:ARG:NH1	1.61	1.00
1:I:228[A]:ARG:HH11	1:I:228[A]:ARG:HG3	0.80	0.92
1:L:154:ILE:HD13	1:L:170:VAL:HG22	1.60	0.84
1:J:237:ARG:O	1:J:238:THR:HG22	1.81	0.80
1:J:154:ILE:HD13	1:J:170:VAL:HG22	1.65	0.79
1:G:207:VAL:HG13	1:G:208:LEU:HD13	1.68	0.76
1:I:144:LEU:HD22	1:I:208:LEU:CD1	2.16	0.76
1:J:207:VAL:HG13	1:J:208:LEU:HD12	1.67	0.74
1:I:144:LEU:HD22	1:I:208:LEU:HD13	1.70	0.74
1:K:154:ILE:HD13	1:K:170:VAL:HG22	1.70	0.73
1:G:159:VAL:HG21	1:G:164:ARG:CZ	2.18	0.73
1:L:147:THR:HG22	1:L:156:CYS:SG	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:VAL:HG21	1:I:233:LEU:HD21	1.74	0.68
1:G:192:ILE:HD12	1:G:225:ASP:HB3	1.77	0.66
1:D:183:ILE:HD13	1:D:233:LEU:HD11	1.79	0.62
1:D:183:ILE:HD13	1:D:233:LEU:CD1	2.28	0.62
1:B:157:PHE:HE2	1:B:204[A]:ILE:HD11	1.64	0.62
1:J:154:ILE:CD1	1:J:170:VAL:HG22	2.32	0.60
1:G:204:ILE:HA	1:G:207:VAL:HG12	1.84	0.59
1:J:169:GLN:O	1:J:173:SER:HB3	2.03	0.59
1:F:186:VAL:HG21	1:F:233:LEU:HD21	1.84	0.58
1:H:186:VAL:HG21	1:H:233:LEU:HD21	1.86	0.57
1:B:157:PHE:CE2	1:B:204[A]:ILE:HD11	2.39	0.57
1:L:144:LEU:HD21	1:L:208:LEU:HD22	1.86	0.57
1:I:144:LEU:N	2:I:291:HOH:O	2.38	0.56
1:A:147:THR:HG22	1:A:156[A]:CYS:SG	2.46	0.56
1:C:142:THR:O	1:C:204:ILE:HD13	2.06	0.56
1:A:144:LEU:HD11	1:A:155:SER:HB3	1.87	0.55
1:G:159:VAL:O	1:G:159:VAL:HG23	2.06	0.55
1:H:153:SER:C	1:H:154:ILE:HD12	2.33	0.53
1:A:145[B]:THR:CG2	1:A:146:GLN:N	2.71	0.53
1:J:171:LEU:HD22	1:J:183:ILE:HG12	1.90	0.53
1:G:171:LEU:HD22	1:G:183:ILE:HD13	1.91	0.51
1:H:178:PHE:HB2	1:H:183:ILE:HD11	1.91	0.51
1:L:192:ILE:HD12	1:L:225:ASP:HB3	1.93	0.51
1:J:197[B]:CYS:SG	1:J:202:LEU:HD13	2.51	0.51
1:K:168:PRO:HA	1:K:171:LEU:HD12	1.93	0.51
1:B:204[A]:ILE:HG22	2:B:318:HOH:O	2.11	0.51
1:F:144:LEU:CD2	1:F:208:LEU:HD12	2.41	0.50
1:K:207:VAL:HG13	1:K:208:LEU:HD12	1.92	0.50
1:L:200:ASP:O	1:L:204:ILE:HD13	2.11	0.50
1:G:159:VAL:HG21	1:G:164:ARG:NE	2.26	0.50
1:K:204:ILE:O	1:K:208:LEU:HD13	2.11	0.50
1:C:185:THR:O	1:C:189:GLU:HG3	2.11	0.49
1:B:211:LEU:HD11	1:B:218:CYS:SG	2.52	0.49
1:K:171:LEU:HD11	1:K:180:LEU:HD13	1.95	0.48
1:F:166:CYS:O	1:F:170:VAL:HG23	2.14	0.48
1:J:204:ILE:O	1:J:207:VAL:HG12	2.13	0.48
1:I:206:LYS:NZ	1:I:215:ALA:HB3	2.28	0.48
1:L:186:VAL:HG21	1:L:233:LEU:HD21	1.95	0.48
1:F:144:LEU:HD11	1:F:155:SER:HB3	1.94	0.48
1:K:171:LEU:CD1	1:K:180:LEU:HD13	2.44	0.48
1:I:153:SER:C	1:I:154:ILE:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:GLN:O	1:E:185:THR:HG22	2.15	0.47
1:J:186:VAL:HG21	1:J:233:LEU:HD21	1.96	0.47
1:C:186:VAL:HG21	1:C:233:LEU:HD21	1.95	0.47
1:C:145:THR:HG23	1:C:156:CYS:SG	2.54	0.47
1:I:206:LYS:HZ3	1:I:215:ALA:HB3	1.80	0.47
1:K:192:ILE:HD12	1:K:225:ASP:HB3	1.97	0.47
1:E:164[A]:ARG:HD3	1:E:222:THR:HG22	1.96	0.47
1:K:192:ILE:HD12	1:K:225:ASP:CG	2.40	0.47
1:F:197:CYS:SG	1:F:218:CYS:HB3	2.55	0.47
1:B:142:THR:O	1:B:204[A]:ILE:HD13	2.15	0.46
1:A:203:HIS:O	1:A:207:VAL:HG13	2.14	0.46
1:F:152:GLU:HG2	1:F:173:SER:HB3	1.97	0.46
1:H:153:SER:O	1:H:154:ILE:HD12	2.14	0.46
1:F:164:ARG:HB3	1:F:220:LEU:HB3	1.98	0.46
1:K:169:GLN:NE2	1:K:210:ILE:HD12	2.30	0.46
1:L:154:ILE:CD1	1:L:170:VAL:HG22	2.39	0.46
1:L:149:LEU:HB3	1:L:154:ILE:HD12	1.98	0.46
1:L:192:ILE:HD12	1:L:225:ASP:CB	2.46	0.46
1:C:192:ILE:HG23	1:C:225:ASP:HB3	1.98	0.45
1:H:171:LEU:HD23	1:H:180:LEU:HD13	1.98	0.45
1:D:211:LEU:HD11	1:D:218:CYS:SG	2.57	0.45
1:G:192:ILE:HD12	1:G:225:ASP:CB	2.46	0.44
1:I:206:LYS:HZ2	1:I:213:PHE:C	2.25	0.44
1:K:186:VAL:HG21	1:K:233:LEU:HD21	1.99	0.44
1:E:231:ASN:HB2	2:E:348:HOH:O	2.18	0.44
1:G:211:LEU:HD11	1:G:218:CYS:SG	2.58	0.44
1:H:144:LEU:HD11	1:H:155:SER:HB3	2.00	0.44
1:K:192:ILE:HD12	1:K:225:ASP:CB	2.48	0.44
1:E:180:LEU:HD23	1:E:184:ASN:ND2	2.32	0.44
1:F:167:LEU:HB3	1:F:168:PRO:HD3	2.00	0.44
1:I:228[A]:ARG:CG	1:I:228[A]:ARG:NH1	2.41	0.44
1:J:173:SER:O	1:J:176:ARG:HG3	2.18	0.44
1:I:144:LEU:HD22	1:I:208:LEU:HD12	1.96	0.43
1:A:192:ILE:HD12	1:A:225:ASP:HB3	2.01	0.43
1:E:211:LEU:HD11	1:E:218:CYS:SG	2.58	0.43
1:B:145:THR:HG23	1:B:156:CYS:SG	2.59	0.43
1:I:203:HIS:O	1:I:207:VAL:HG23	2.19	0.43
1:E:228:ARG:C	2:E:348:HOH:O	2.61	0.43
1:F:142:THR:O	1:F:142:THR:HG23	2.19	0.43
1:K:149:LEU:HB3	1:K:154:ILE:HD12	2.00	0.43
1:K:182:GLN:O	1:K:186:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD13	1:B:233:LEU:HD11	2.01	0.42
1:J:154:ILE:HD13	1:J:170:VAL:CG2	2.42	0.42
1:E:178:PHE:HB2	1:E:183:ILE:HD11	2.02	0.42
1:D:173:SER:OG	1:D:174:VAL:N	2.53	0.41
1:L:147:THR:CG2	1:L:156:CYS:SG	3.05	0.41
1:C:186:VAL:HG21	1:C:233:LEU:CD2	2.50	0.41
1:J:237:ARG:O	1:J:238:THR:CG2	2.60	0.41
1:L:192:ILE:HD12	1:L:225:ASP:CG	2.46	0.41
1:I:144:LEU:CD2	1:I:208:LEU:HD13	2.46	0.41
1:G:145:THR:HG23	1:G:156:CYS:SG	2.60	0.41
1:G:144:LEU:HD13	1:G:157:PHE:CZ	2.55	0.41
1:I:152:GLU:HG2	1:I:173:SER:HB3	2.03	0.41
1:I:214[A]:ASN:HD22	1:I:214[A]:ASN:HA	1.71	0.40
1:K:144:LEU:HD13	1:K:157:PHE:CZ	2.57	0.40
1:G:158:GLN:NE2	1:G:160:GLY:O	2.54	0.40
1:G:174:VAL:HG12	1:G:175:LEU:HD23	2.03	0.40
1:E:182:GLN:HA	1:E:185:THR:HG22	2.03	0.40
1:J:167:LEU:HB3	1:J:168:PRO:HD3	2.03	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	103/125 (82%)	101 (98%)	2 (2%)	0	100	100
1	B	100/125 (80%)	98 (98%)	2 (2%)	0	100	100
1	C	95/125 (76%)	92 (97%)	3 (3%)	0	100	100
1	D	95/125 (76%)	90 (95%)	5 (5%)	0	100	100
1	E	94/125 (75%)	92 (98%)	2 (2%)	0	100	100
1	F	98/125 (78%)	92 (94%)	5 (5%)	1 (1%)	12	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	93/125 (74%)	89 (96%)	4 (4%)	0	100	100
1	H	96/125 (77%)	91 (95%)	5 (5%)	0	100	100
1	I	95/125 (76%)	91 (96%)	4 (4%)	0	100	100
1	J	95/125 (76%)	92 (97%)	3 (3%)	0	100	100
1	K	95/125 (76%)	94 (99%)	1 (1%)	0	100	100
1	L	93/125 (74%)	91 (98%)	2 (2%)	0	100	100
All	All	1152/1500 (77%)	1113 (97%)	38 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	142	THR

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	97/115 (84%)	94 (97%)	3 (3%)	35	50
1	B	94/115 (82%)	94 (100%)	0	100	100
1	C	90/115 (78%)	89 (99%)	1 (1%)	65	76
1	D	89/115 (77%)	89 (100%)	0	100	100
1	E	88/115 (76%)	86 (98%)	2 (2%)	44	59
1	F	92/115 (80%)	92 (100%)	0	100	100
1	G	87/115 (76%)	86 (99%)	1 (1%)	65	76
1	H	90/115 (78%)	89 (99%)	1 (1%)	65	76
1	I	89/115 (77%)	84 (94%)	5 (6%)	19	27
1	J	89/115 (77%)	87 (98%)	2 (2%)	45	60
1	K	89/115 (77%)	89 (100%)	0	100	100
1	L	87/115 (76%)	86 (99%)	1 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1081/1380 (78%)	1065 (98%)	16 (2%)	61 70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	GLU
1	A	189	GLU
1	A	207	VAL
1	C	208	LEU
1	E	180	LEU
1	E	204	ILE
1	G	208	LEU
1	H	183	ILE
1	I	196	ARG
1	I	214[A]	ASN
1	I	214[B]	ASN
1	I	228[A]	ARG
1	I	228[B]	ARG
1	J	143	GLU
1	J	238	THR
1	L	197	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	184	ASN
1	E	231	ASN
1	F	181	GLN
1	I	146	GLN
1	K	181	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	102/125 (81%)	0.15	4 (3%) 43 43	1, 4, 4, 5	4 (3%)
1	B	97/125 (77%)	0.04	1 (1%) 79 80	2, 4, 5, 5	6 (6%)
1	C	97/125 (77%)	-0.15	1 (1%) 79 80	2, 4, 5, 5	1 (1%)
1	D	96/125 (76%)	-0.08	1 (1%) 79 80	2, 4, 4, 5	2 (2%)
1	E	95/125 (76%)	0.20	2 (2%) 63 65	2, 4, 4, 4	1 (1%)
1	F	98/125 (78%)	-0.05	3 (3%) 51 52	2, 4, 4, 5	2 (2%)
1	G	95/125 (76%)	0.23	3 (3%) 50 51	3, 4, 4, 4	0
1	H	96/125 (76%)	0.05	0 100 100	2, 4, 4, 5	2 (2%)
1	I	94/125 (75%)	0.31	4 (4%) 40 39	2, 4, 5, 7	4 (4%)
1	J	96/125 (76%)	0.85	17 (17%) 4 3	2, 4, 5, 5	1 (1%)
1	K	96/125 (76%)	0.21	1 (1%) 79 80	2, 4, 4, 4	2 (2%)
1	L	94/125 (75%)	0.12	3 (3%) 50 51	2, 4, 4, 5	2 (2%)
All	All	1156/1500 (77%)	0.16	40 (3%) 47 47	1, 4, 4, 7	27 (2%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	190	LEU	5.8
1	J	221	ILE	3.8
1	A	174	VAL	3.5
1	J	192	ILE	3.5
1	J	222	THR	3.4
1	J	191	TYR	3.4
1	E	199	SER	3.3
1	J	146	GLN	3.3
1	F	238	THR	3.3
1	J	238	THR	3.1
1	E	180	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	216	PRO	2.9
1	J	193	TYR	2.8
1	J	223	LEU	2.8
1	J	143	GLU	2.8
1	I	159	VAL	2.7
1	K	202	LEU	2.7
1	I	163	LYS	2.6
1	J	214	ASN	2.6
1	A	189	GLU	2.6
1	L	163	LYS	2.6
1	J	189	GLU	2.6
1	I	158	GLN	2.6
1	G	160	GLY	2.5
1	C	141	SER	2.5
1	L	160	GLY	2.5
1	D	143	GLU	2.4
1	J	144	LEU	2.3
1	J	213	PHE	2.3
1	J	185	THR	2.3
1	F	141	SER	2.3
1	A	197[A]	CYS	2.3
1	B	237	ARG	2.3
1	J	187	CYS	2.2
1	A	196	ARG	2.1
1	J	199	SER	2.1
1	G	142	THR	2.1
1	G	198	THR	2.0
1	I	161	GLY	2.0
1	L	161	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.