



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:50 am BST

PDB ID : 3S51
Title : Structure of FANCI
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

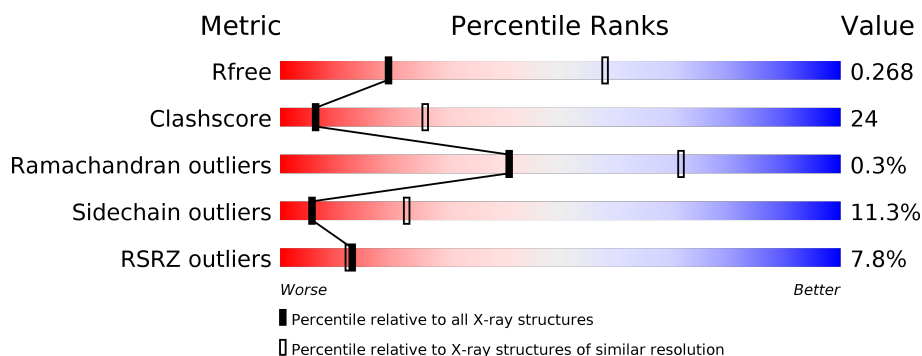
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	1308	<div> <div>6%</div> <div>44%</div> <div>37%</div> <div>5%</div> <div>13%</div> </div>
1	B	1308	<div> <div>8%</div> <div>41%</div> <div>36%</div> <div>5%</div> <div>18%</div> </div>
1	C	1308	<div> <div>5%</div> <div>45%</div> <div>37%</div> <div>5%</div> <div>13%</div> </div>
1	D	1308	<div> <div>6%</div> <div>40%</div> <div>34%</div> <div>5%</div> <div>21%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34594 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 Fanconi anemia group I protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	B	1071	Total	C	N	O	S	0	0	0
			8487	5468	1409	1559	51			
1	C	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	D	1034	Total	C	N	O	S	0	0	0
			8187	5277	1358	1504	48			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1305	HIS	-	EXPRESSION TAG	UNP Q8K368

Continued on next page...

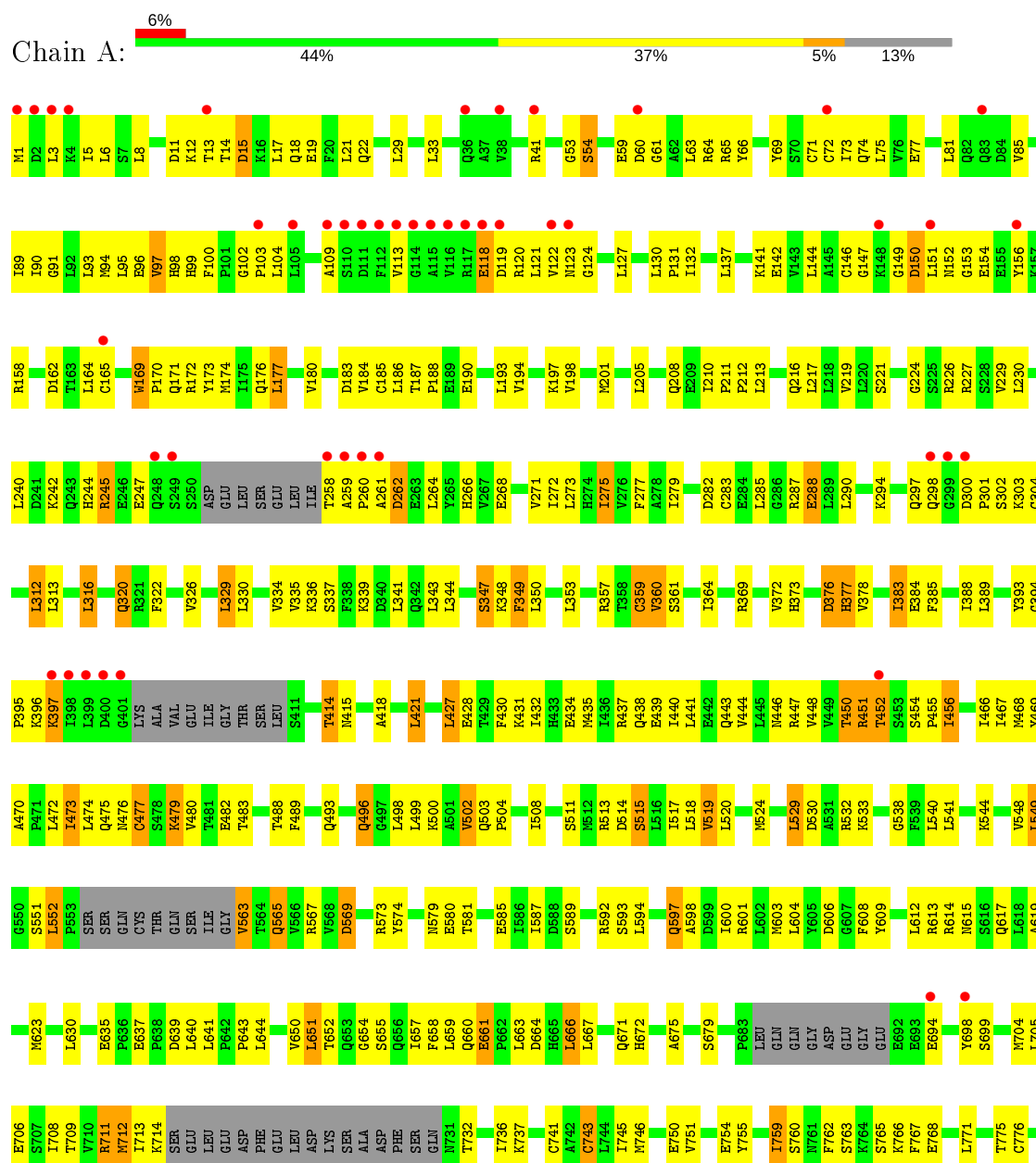
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1308	HIS	-	EXPRESSION TAG	UNP Q8K368

3 Residue-property plots

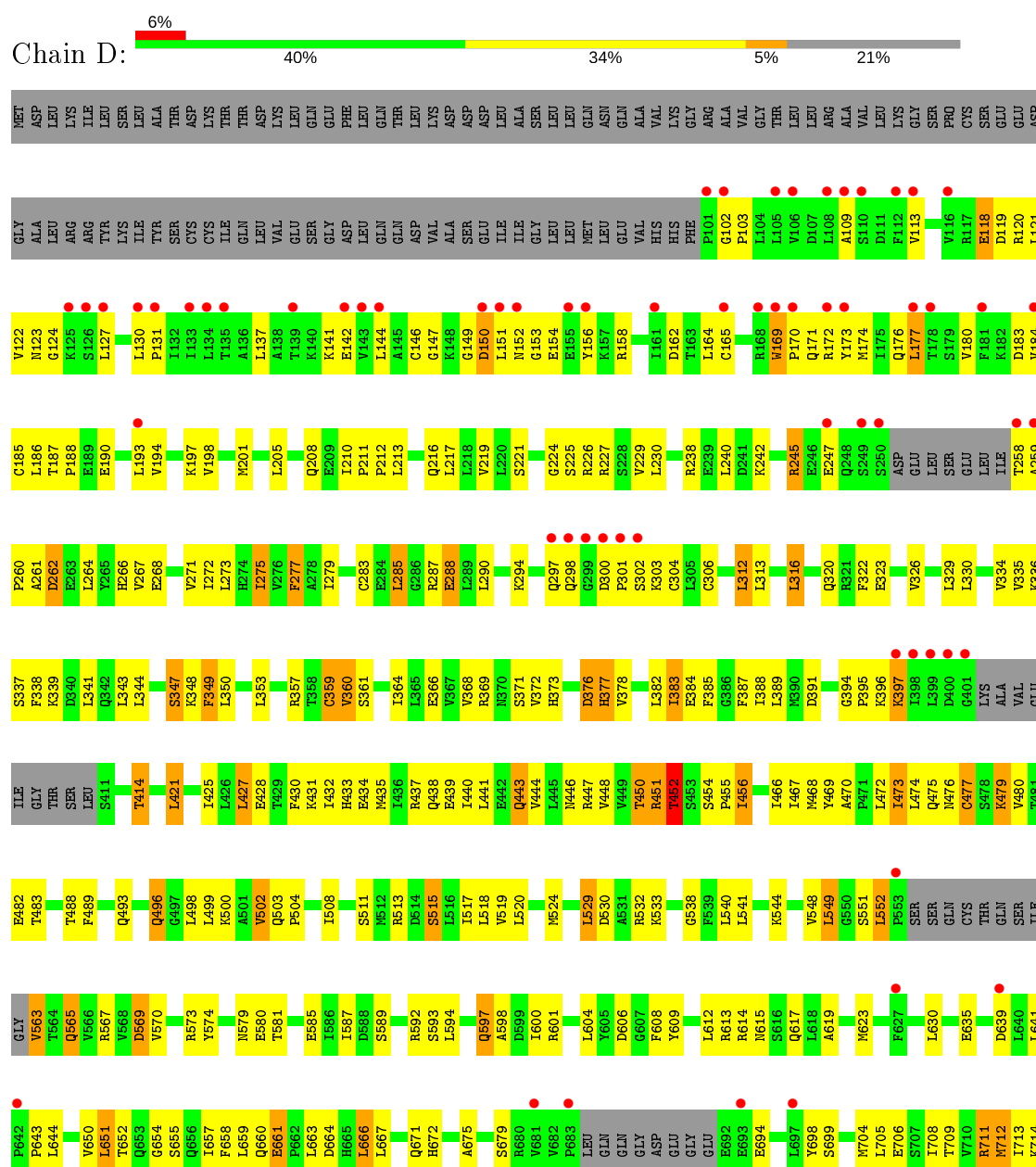
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Fanconi anemia group I protein homolog





T995	F915	F837	S765	GLU	R613	P539	S454	I388	P301	G224	G149	E77	M1
S996	V918	M638	K766	E892	R614	L540	P456	L389	S302	G224	D150	L81	D2
Q998	L919	H839	F767	E694	R615	L541	I456	M390	K303	R226	N152	L81	L3
F999	L919	Y840	E768	E694	S616	K544	I466	D391	C304	R226	G153	D84	K4
V1000	Y922	N843	L771	Y698	L617	K544	I467	G384	L312	V229	E154	D84	L5
Q1001	Q923	Q923	S772	S699	L618	V543	M468	P395	L313	L230	E155	S7	L6
H1002	P924	L846	T775	M704	A619	L549	M468	P396	L316	L240	Y156	L89	L8
S1003	C776	Q847	C776	L705	M623	S551	M468	P396	L316	L240	Y156	I90	A9
W1005	L930	L852	C776	E706	F627	S551	M468	P396	L316	L240	Y156	I90	T10
I1009	Q931	I853	K779	S707	L630	P563	M468	P396	Q320	K242	D162	L92	D11
E934	V858	V858	F780	I708	L630	SER	M468	P396	R321	R245	G165	L93	K12
Y1013	S859	S859	I783	I710	K631	SER	M468	P396	F322	E246	E168	L94	T13
S1014	NET	G860	L784	R711	K631	GLN	M468	P396	V326	E247	R168	E96	T14
G1019	GLY	P861	SER	R712	E635	CYS	M468	P396	L329	ASP	W169	K16	D15
F1020	THR	D862	GLU	M713	P636	THR	M468	P396	L329	ASP	W169	K16	L17
C1021	GLU	K714	LYS	K714	E637	GLN	M468	P396	L330	GLU	P170	L17	L18
K1022	GLU	SER	ALA	SER	P638	SER	M468	P396	L330	GLU	Q171	L19	E19
S1023	GLU	GLY	GLY	ILE	D639	ILE	M468	P396	V334	SER	R172	F101	F20
L1024	ALA	GLY	GLY	V563	L641	THR	M468	P396	V335	GLU	M174	P101	L21
F1029	GLY	F870	GLY	T564	P642	GLY	M468	P396	K336	LEU	Q175	L104	Q22
S1030	V945	Q871	ALA	Q565	P643	Q565	M468	P396	S337	ILE	L177	L106	D28
L1031	T946	N872	LYS	D569	L644	D569	M468	P396	K339	A259	L180	L106	L29
H1032	V947	T877	THR	V570	V650	V570	M468	P396	L341	A261	Y180	L109	L33
V1033	Q949	R878	SER	R573	L651	R573	M468	P396	L341	A261	Y180	L109	L33
L1034	R950	R879	SER	Y574	T652	Y574	M468	P396	Q342	D263	D183	S110	Q36
Y1035	A951	L880	ALA	G654	G653	G654	M468	P396	L343	E263	V184	F112	A37
S952	S952	L881	ASP	S655	G654	S655	M468	P396	L344	E263	C185	V113	V38
F953	D801	W882	ASP	G656	G656	G656	M468	P396	S347	H266	L186	G114	R41
Q954	S803	S803	SER	F658	F658	F658	M468	P396	F349	E267	P188	V116	A42
S1046	S803	S803	GLN	T581	T581	T581	M468	P396	L350	E268	E189	R117	A42
I1049	Q957	S886	ILE	E585	N731	E585	M468	P396	L350	E268	E189	E118	L47
H1050	P900	P900	THR	I587	I732	I587	M468	P396	L353	L272	L193	D119	R48
L1053	L812	L812	SER	D588	I736	D588	M468	P396	R357	I275	V194	R120	L51
G1054	T814	T814	VAL	S589	K737	S589	M468	P396	R357	I275	V194	L121	L51
D1055	A815	A815	GLU	R592	C741	R592	M468	P396	T358	V276	K197	L122	R52
I1056	L816	L816	GLU	S593	C742	S593	M468	P396	C359	F277	N123	G124	G53
ASP	R817	R817	SER	L594	C743	L594	M468	P396	V360	A278	V198	G124	S54
GLN	R818	R818	GLY	L594	L744	L594	M468	P396	S361	I279	W201	K125	S54
ASP	D819	D819	LYS	Q597	M746	Q597	M468	P396	I364	C283	L205	L127	E59
ASP	H824	H824	LYS	L516	V751	L516	M468	P396	I364	C283	L205	L127	D60
VAL	E825	E825	LYS	A598	L752	A598	M468	P396	V368	E284	L205	L130	G61
GLU	E826	E826	LYS	D599	L753	D599	M468	P396	V368	E284	L205	L130	A62
ILE	S827	S827	LYS	L600	H753	L600	M468	P396	V368	E284	L205	L130	L63
GLU	S828	S828	LYS	L601	L754	L601	M468	P396	V368	E284	L205	L130	L63
LYS	S829	S829	LYS	L602	Y755	L602	M468	P396	V368	E284	L205	L130	R64
THR	S830	S830	LYS	L603	Y755	L603	M468	P396	V368	E284	L205	L130	R65
ASP	L831	L831	LYS	L604	Y755	L604	M468	P396	V368	E284	L205	L130	R65
HIS	R832	R832	LYS	L605	Y755	L605	M468	P396	V368	E284	L205	L130	Y66
PHE	S833	S833	LYS	L606	Y755	L606	M468	P396	V368	E284	L205	L130	Y66
ALA	S834	S834	LYS	L607	Y755	L607	M468	P396	V368	E284	L205	L130	Y66
V1070	V1071	V1071	LYS	L608	Y755	L608	M468	P396	V368	E284	L205	L130	Y66
V1071	V1071	V1071	LYS	L609	Y755	L609	M468	P396	V368	E284	L205	L130	Y66
A1076	A1076	A1076	LYS	L610	Y755	L610	M468	P396	V368	E284	L205	L130	Y66
				L611	Y755	L611	M468	P396	V368	E284	L205	L130	Y66
				L612	Y755	L612	M468	P396	V368	E284	L205	L130	Y66
				L613	Y755	L613	M468	P396	V368	E284	L205	L130	Y66
				L614	Y755	L614	M468	P396	V368	E284	L205	L130	Y66
				L615	Y755	L615	M468	P396	V368	E284	L205	L130	Y66
				L616	Y755	L616	M468	P396	V368	E284	L205	L130	Y66
				L617	Y755	L617	M468	P396	V368	E284	L205	L130	Y66
				L618	Y755	L618	M468	P396	V368	E284	L205	L130	Y66
				L619	Y755	L619	M468	P396	V368	E284	L205	L130	Y66
				L620	Y755	L620	M468	P396	V368	E284	L205	L130	Y66
				L621	Y755	L621	M468	P396	V368	E284	L205	L130	Y66
				L622	Y755	L622	M468	P396	V368	E284	L205	L130	Y66
				L623	Y755	L623	M468	P396	V368	E284	L205	L130	Y66
				L624	Y755	L624	M468	P396	V368	E284	L205	L130	Y66
				L625	Y755	L625	M468	P396	V368	E284	L205	L130	Y66
				L626	Y755	L626	M468	P396	V368	E284	L205	L130	Y66
				L627	Y755	L627	M468	P396	V368	E284	L205	L130	Y66
				L628	Y755	L628	M468	P396	V368	E284	L205	L130	Y66
				L629	Y755	L629	M468	P396	V368	E284	L205	L130	Y66
				L630	Y755	L630	M468	P396	V368	E284	L205	L130	Y66
				L631	Y755	L631	M468	P396	V368	E284	L205	L130	Y66
				L632	Y755	L632	M468	P396	V368	E284	L205	L130	Y66
				L633	Y755	L633	M468	P396	V368	E284	L205	L130	Y66
				L634	Y755	L634	M468	P396	V368	E284	L205	L130	Y66
				L635	Y755	L635	M468	P396	V368	E284	L205	L130	Y66
				L636	Y755	L636	M468	P396	V368	E284	L205	L130	Y66
				L637	Y755	L637	M468	P396	V368	E284	L205	L130	Y66
				L638	Y755	L638	M468	P396	V368	E284	L205	L130	Y66
				L639	Y755	L639	M468	P396	V368	E284	L205	L130	Y66
				L640	Y755	L640	M468	P396	V368	E284	L205	L130	Y66
				L641	Y755	L641	M468	P396	V368	E284	L205	L130	Y66
				L642	Y755	L642	M468	P396	V368	E284	L205	L130	Y66
				L643	Y755	L643	M468	P396	V368	E284	L205	L130	Y66
				L644	Y755	L644	M468	P396	V368	E284	L205	L130	Y66
				L645	Y755	L645	M468	P396	V368	E284	L205	L130	Y66
				L646	Y755	L646	M468	P396	V368	E284	L205	L130	Y66
				L647	Y755	L647	M468	P396	V368	E284	L205	L130	Y66
				L648	Y755	L648	M468	P396	V368	E284	L205	L130	Y66
				L649	Y755	L649	M468	P396	V368	E284	L205	L130	Y66
				L650	Y755	L650	M468	P396	V368	E284	L205	L130	Y66
				L651	Y755	L651	M468	P396	V368	E284	L205	L130	Y66
				L652	Y755	L652	M468	P396	V368	E284	L205	L130	Y66
				L653	Y755	L653	M468	P396	V368	E284	L205	L130	Y66
				L654	Y755	L654	M468	P396	V368	E284	L205	L130	Y66
				L655	Y755	L655	M468	P396	V368	E284	L205	L130	Y66
				L656	Y755	L656	M468	P396	V368	E284	L205	L130	Y66
				L657	Y755	L657	M468	P396	V368	E284	L205	L130	Y66
				L658	Y755	L658	M468	P396	V368	E284	L205	L130	Y66
				L659	Y755	L659	M468	P396	V368	E284	L205	L130	Y66
				L660	Y755	L660	M468	P396	V368	E284	L205	L130	Y66
				L661	Y755	L661	M468	P396	V368	E284	L205	L130	Y66
				L662	Y755	L662	M468	P396	V368	E284	L205	L130	Y66
				L663	Y755	L663	M468	P396	V368	E284	L205	L130	Y66
				L664	Y755	L664	M468	P396	V368	E284	L205	L130	Y66
				L665	Y755	L665	M468	P396	V368	E284	L205	L130	Y66
				L666	Y755	L666	M468	P396	V368	E284	L205	L130	Y66
				L667	Y755	L667	M468	P396	V368	E284	L205	L130	Y66
				L668	Y755	L668	M468	P396	V368	E284	L205	L130	Y66
				L669	Y755	L669	M468	P396	V368	E284	L205	L130	Y66
				L670	Y755	L670	M468	P396	V368	E284	L205	L130	Y66
				L671	Y755	L671	M468</						





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.70 Å 136.50 Å 149.70 Å 115.90° 106.00° 95.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.28	Depositor EDS
% Data completeness (in resolution range)	82.8 (39.82-3.30) 83.1 (39.82-3.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.25 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.259 , 0.278 0.245 , 0.268	Depositor DCC
R_{free} test set	2199 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 117.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34594	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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	0.26	2/9099 (0.0%)	0.46	0/12286
1	B	0.29	4/8624 (0.0%)	0.46	0/11646
1	C	0.26	2/9099 (0.0%)	0.46	0/12286
1	D	0.26	2/8319 (0.0%)	0.46	0/11234
All	All	0.27	10/35141 (0.0%)	0.46	0/47452

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	959	GLN	CD-NE2	-9.98	1.07	1.32
1	B	959	GLN	CD-OE1	-7.80	1.06	1.24
1	C	320	GLN	CD-NE2	-6.76	1.16	1.32
1	D	320	GLN	CD-NE2	-6.59	1.16	1.32
1	A	320	GLN	CD-NE2	-6.15	1.17	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide
1	B	1053	LEU	Peptide
1	C	1053	LEU	Peptide
1	D	1053	LEU	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	8960	0	9275	454	0
1	B	8487	0	8776	449	0
1	C	8960	0	9275	435	0
1	D	8187	0	8476	411	0
All	All	34594	0	35802	1705	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 24.

The worst 5 of 1705 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:C:799:VAL:O	1:C:847:GLN:NE2	1.87	1.07
1:A:799:VAL:O	1:A:847:GLN:NE2	1.88	1.07
1:B:799:VAL:O	1:B:847:GLN:NE2	1.88	1.06
1:D:799:VAL:O	1:D:847:GLN:NE2	1.88	1.05
1:A:489:PHE:HB3	1:C:450:THR:HG21	1.35	1.04

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	1108/1308 (85%)	1023 (92%)	82 (7%)	3 (0%)	41	71
1	B	1045/1308 (80%)	969 (93%)	72 (7%)	4 (0%)	34	66
1	C	1108/1308 (85%)	1022 (92%)	83 (8%)	3 (0%)	41	71
1	D	1008/1308 (77%)	933 (93%)	71 (7%)	4 (0%)	34	66
All	All	4269/5232 (82%)	3947 (92%)	308 (7%)	14 (0%)	41	71

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	B	122	VAL
1	B	150	ASP
1	C	122	VAL

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	1032/1188 (87%)	917 (89%)	115 (11%)	6	23
1	B	979/1188 (82%)	867 (89%)	112 (11%)	5	22
1	C	1032/1188 (87%)	917 (89%)	115 (11%)	6	23
1	D	945/1188 (80%)	838 (89%)	107 (11%)	6	22
All	All	3988/4752 (84%)	3539 (89%)	449 (11%)	6	22

5 of 449 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	878	ARG
1	C	288	GLU
1	D	765	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	981	LEU
1	C	19	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	433	HIS
1	B	672	HIS
1	D	433	HIS
1	B	377	HIS
1	D	377	HIS

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 carbohydrates 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	1134/1308 (86%)	0.25	85 (7%) 14 13	85, 192, 306, 410	0
1	B	1071/1308 (81%)	0.27	101 (9%) 8 9	87, 188, 306, 415	0
1	C	1134/1308 (86%)	0.25	70 (6%) 20 20	81, 191, 306, 410	0
1	D	1034/1308 (79%)	0.28	84 (8%) 12 11	84, 185, 302, 416	0
All	All	4373/5232 (83%)	0.26	340 (7%) 13 12	81, 189, 304, 416	0

The worst 5 of 340 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	ALA	12.3
1	D	250	SER	11.1
1	D	135	THR	10.9
1	D	150	ASP	8.9
1	D	299	GLY	8.7

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 carbohydrates 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.