



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 05:40 PM EDT

PDB ID : 3H7N / pdb_00003h7n
Title : Structure of Nup120
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Deposited on : 2009-04-27
Resolution : 3.00 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

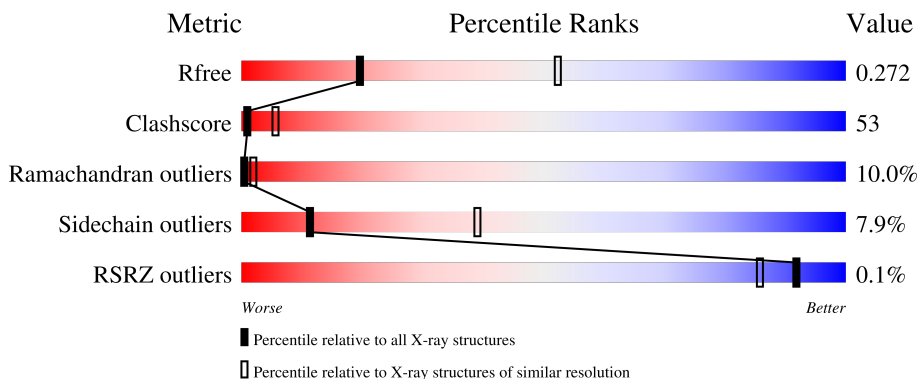
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	729	
1	B	729	
1	C	729	
1	D	729	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22992 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.

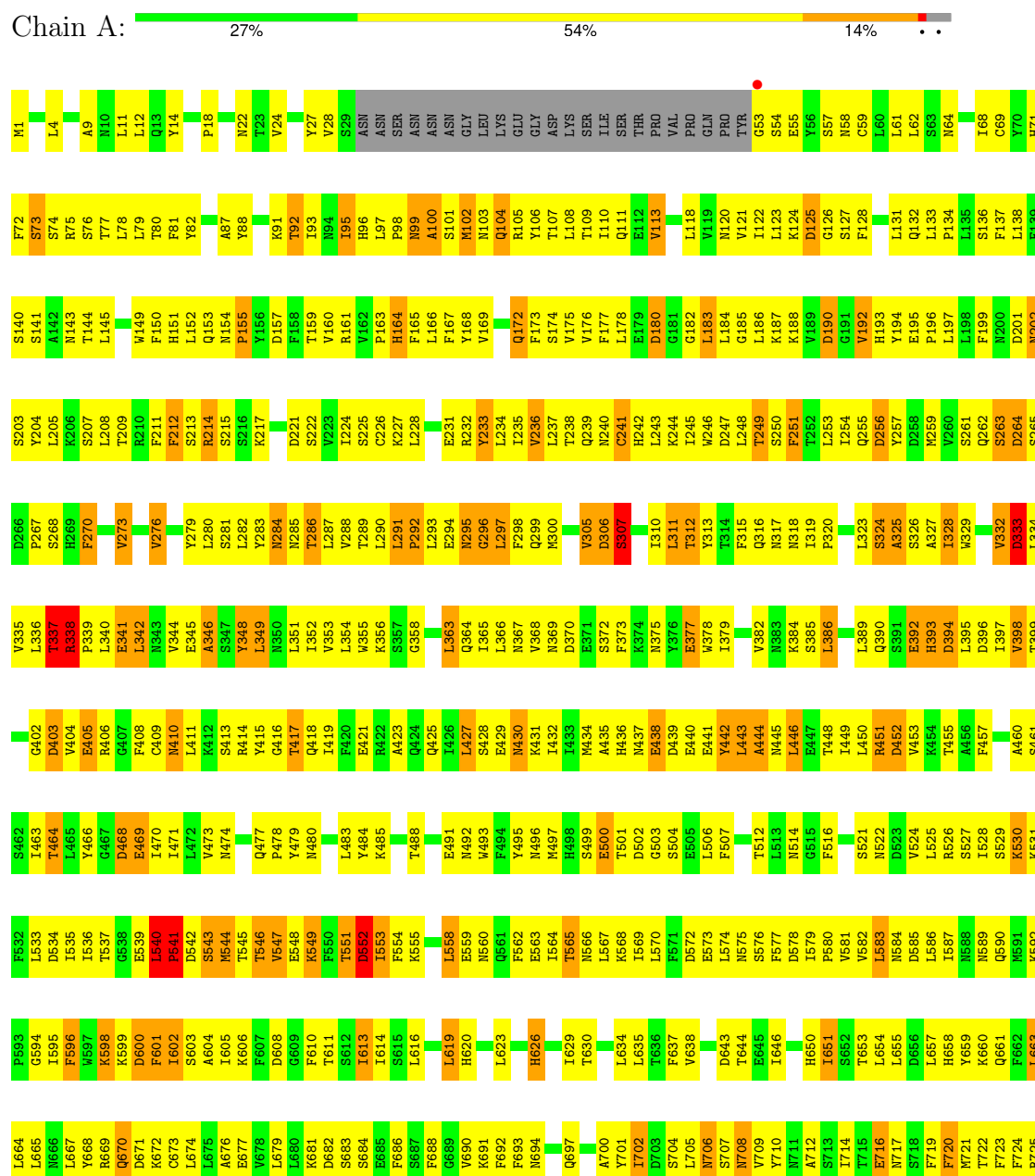
- Molecule 1 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			
1	B	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			
1	C	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			
1	D	706	Total	C	N	O	S	0	0	0
			5748	3718	913	1099	18			

3 Residue-property plots

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.

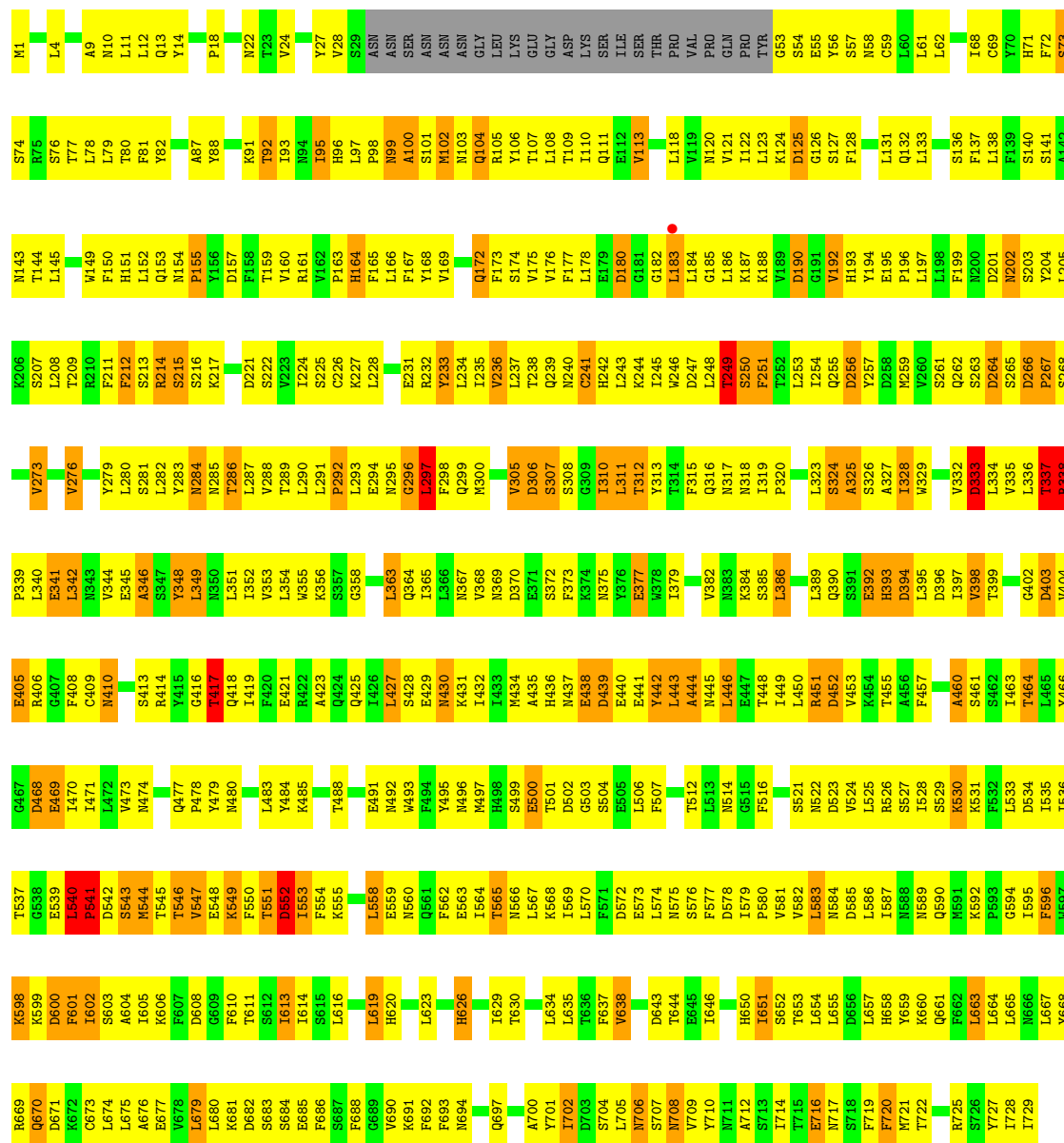
• Molecule 1: Nucleoporin NUP120



S726
Y727
I728
I729

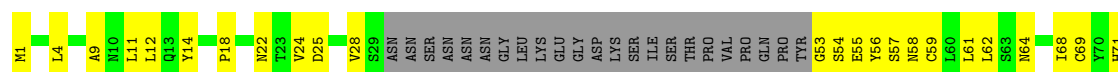
• Molecule 1: Nucleoporin NUP120

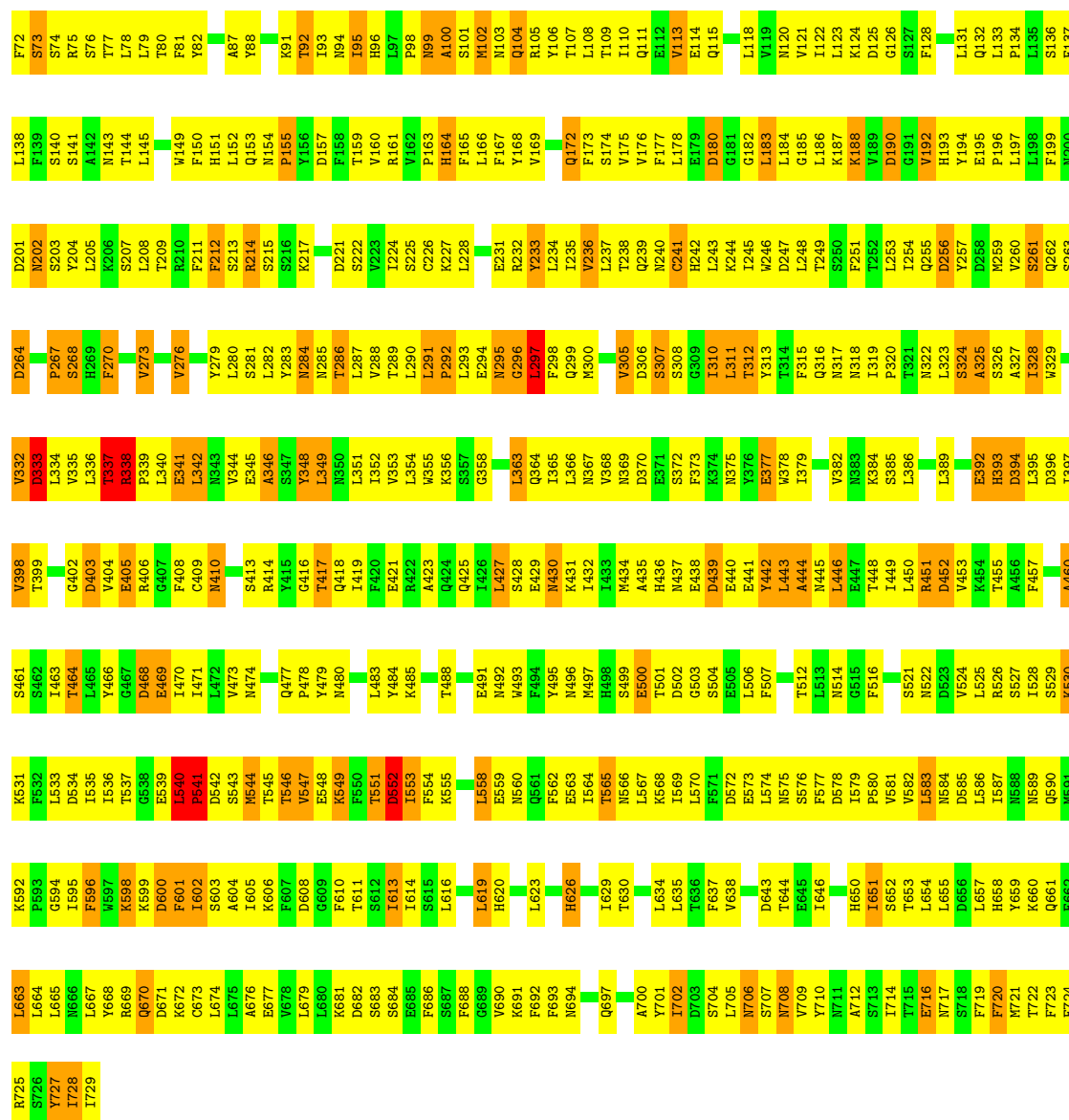
Chain B: 27% 54% 14% ..



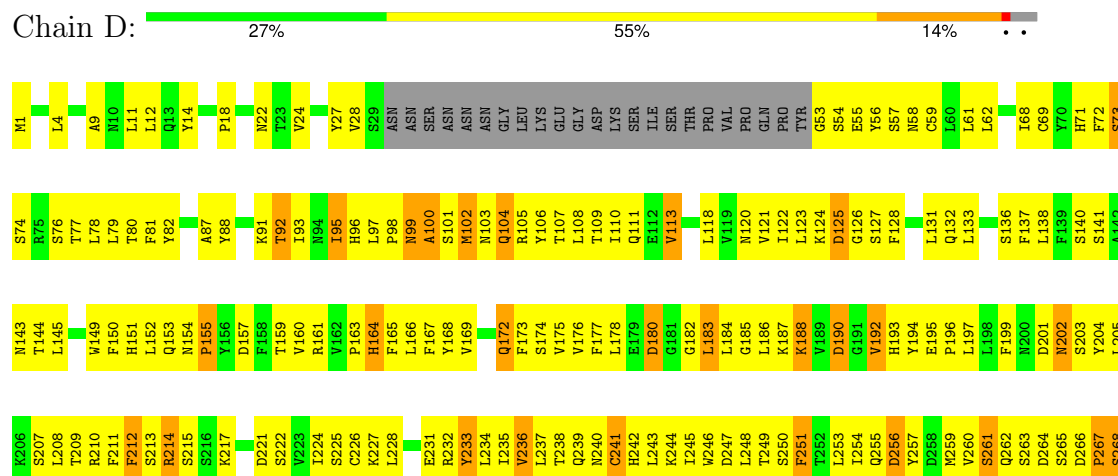
• Molecule 1: Nucleoporin NUP120

Chain C: 27% 55% 14% ..





• Molecule 1: Nucleoporin NUP120



I729	L667	K598	T537	G487	V404	T337	H269
Y668	K599	K598	E538	D468	E405	R338	
R669	D600	E539	E539	E469	R406	P339	V273
Q670	F601	L540	L540	I470	G407	L340	
D671	I602	P541	P541	F408	F408	E341	V276
K672	S603	D542	D542	I471	C409	L342	
C673	A604	S543	S543	L472	M410	K343	Y279
L674	L605	R544	R544	V473		V344	L280
L675	K606	T545	T545	N474	S413	E345	S281
A676	F607	T546	T546	Q477	R414	A346	L282
E677	D608	V547	V547	P478		S347	Y283
V678	G609	E548	E548	Y479	T417	Y348	N284
L679	F610	K549	K549	N480	Q418	N285	N285
L680	T611	F550	F550		I419	T286	
K681	S612	T551	T551	L483	F420	L287	L287
D682	L613	D552	D552	Y484	E421	I352	V288
S683	I614	I553	I553	K485	R422	V353	T289
S684	S615	F554	F554		A423	L354	L290
S685	L616	K555	K555	T488	Q424	K355	L291
F686					Q425	K356	P292
S687	L619	L558	L558	E491	I426	S357	L293
F688	H620	E559	E559	N492	L427	G358	E294
G689		N560	N560	W493	S428		N295
V690	L623	Q561	Q561	F494	E429	L363	G296
K691	H626	F562	F562	Y495	N430	Q364	L287
F692		E563	E563	N496	K431	I365	F298
F693		I564	I564	M497	I432	L366	Q299
N694		T565	T565	H498	I433	N367	M300
Q697		N566	N566	S499	M434	V368	
		L567	L567	E500	A435	N369	L304
A700		K568	K568	T501	H436	D370	V305
Y701		I569	I569	D502	N437	E371	D306
I702		L570	L570	G503	E438	S372	S307
D703		F571	F571	S504	D439	F373	S308
S704		D572	D572	E505	E440	K374	G309
F705		E573	E573	L506	E441	N375	I310
L706		L574	L574	F507	Y442	Y376	I311
N706		N575	N575		L443	E377	T312
S707		S576	S576	T512	A444	W378	T313
N708		F577	F577	L513	N445	I379	T314
V709		D578	D578	N514	L446		F315
Y710		I579	I579	G515	E447	V382	Q316
L711		P580	P580	F516	T448	N383	N317
A712		V581	V581		I449	K384	N318
S713		V582	V582	S521	L450	S385	I319
I714		L583	L583	N522	R451	L386	P320
T715		N584	N584	D523	D452		
E716		D585	D585	V524	V453	L389	S324
N717		L586	L586	R525	K454	A325	A325
S718		I587	I587	R526	T455	S326	S326
F719		N588	N588	S527	A456	A327	A327
F720		N589	N589	I528	P457	W329	W329
N721		Q590	Q590	S529			
T722		N591	N591	K530	A460	D396	L328
F723		K592	K592	K531	S461	I397	I397
F724		P593	P593	F532	S462	V398	V332
N725		G594	G594	L533	I463	T399	D333
S726		I595	I595	D534	T464		L334
Y727		F596	F596	I535	Y465	G402	V335
I728		W597	W597	I536	Y466	D403	L336

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.99Å 115.72Å 156.08Å 90.06° 89.96° 90.02°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 85.3 (50.00-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.255 , 0.274 0.254 , 0.272	Depositor DCC
R_{free} test set	3365 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 131.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l 0.449 for -h,k,-l 0.447 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22992	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	0.59	4/5878 (0.1%)	1.06	45/7981 (0.6%)
1	B	0.57	3/5878 (0.1%)	1.06	40/7981 (0.5%)
1	C	0.57	2/5878 (0.0%)	1.06	40/7981 (0.5%)
1	D	0.57	0/5878	1.07	44/7981 (0.6%)
All	All	0.58	9/23512 (0.0%)	1.06	169/31924 (0.5%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	SER	C-O	8.46	1.34	1.24
1	C	310	ILE	CA-C	6.36	1.59	1.52
1	A	306	ASP	CG-OD2	6.04	1.36	1.25
1	A	306	ASP	C-O	5.88	1.32	1.23
1	B	306	ASP	CA-C	5.73	1.60	1.53

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	VAL	N-CA-C	9.61	120.80	111.67
1	A	305	VAL	N-CA-C	9.50	120.70	111.67
1	B	305	VAL	N-CA-C	9.21	120.42	111.67
1	D	308	SER	N-CA-C	-8.67	101.80	111.07
1	D	305	VAL	CB-CA-C	-8.42	101.87	111.80

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	5748	0	5657	630	0
1	B	5748	0	5657	599	0
1	C	5748	0	5657	624	0
1	D	5748	0	5657	603	0
All	All	22992	0	22628	2422	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 53.

The worst 5 of 2422 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:B:224:ILE:HG12	1:B:273:VAL:HG11	1.23	1.20
1:D:224:ILE:HG12	1:D:273:VAL:HG11	1.23	1.15
1:A:224:ILE:HG12	1:A:273:VAL:HG11	1.24	1.14
1:C:224:ILE:HG12	1:C:273:VAL:HG11	1.22	1.14
1:D:398:VAL:HB	1:D:669:ARG:NH1	1.62	1.14

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	702/729 (96%)	463 (66%)	169 (24%)	70 (10%)	0	2
1	B	702/729 (96%)	469 (67%)	159 (23%)	74 (10%)	0	2
1	C	702/729 (96%)	467 (66%)	165 (24%)	70 (10%)	0	2
1	D	702/729 (96%)	469 (67%)	165 (24%)	68 (10%)	0	2
All	All	2808/2916 (96%)	1868 (66%)	658 (23%)	282 (10%)	0	2

5 of 282 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	104	GLN
1	A	113	VAL
1	A	214	ARG
1	A	241	CYS

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	661/682 (97%)	609 (92%)	52 (8%)	11	39
1	B	661/682 (97%)	608 (92%)	53 (8%)	11	38
1	C	661/682 (97%)	609 (92%)	52 (8%)	11	39
1	D	661/682 (97%)	609 (92%)	52 (8%)	11	39
All	All	2644/2728 (97%)	2435 (92%)	209 (8%)	11	39

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	297	LEU
1	C	558	LEU
1	D	596	PHE
1	C	337	THR
1	C	398	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	GLN
1	D	514	ASN
1	C	425	GLN
1	D	492	ASN
1	D	632	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 [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	706/729 (96%)	-0.90	1 (0%) 92 86	51, 121, 174, 188	0
1	B	706/729 (96%)	-0.89	1 (0%) 92 86	54, 121, 174, 188	0
1	C	706/729 (96%)	-0.92	0 100 100	52, 122, 174, 191	0
1	D	706/729 (96%)	-0.85	1 (0%) 92 86	50, 121, 174, 186	0
All	All	2824/2916 (96%)	-0.89	3 (0%) 92 86	50, 122, 174, 191	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	GLY	3.2
1	D	558	LEU	2.7
1	B	183	LEU	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.