



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:30 AM UTC

PDB ID : 3TKN / pdb\_00003tkn  
Title : Structure of the Nup82-Nup159-Nup98 heterotrimer  
Authors : Stuwe, T.T.; Hoelz, A.  
Deposited on : 2011-08-28  
Resolution : 3.40 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

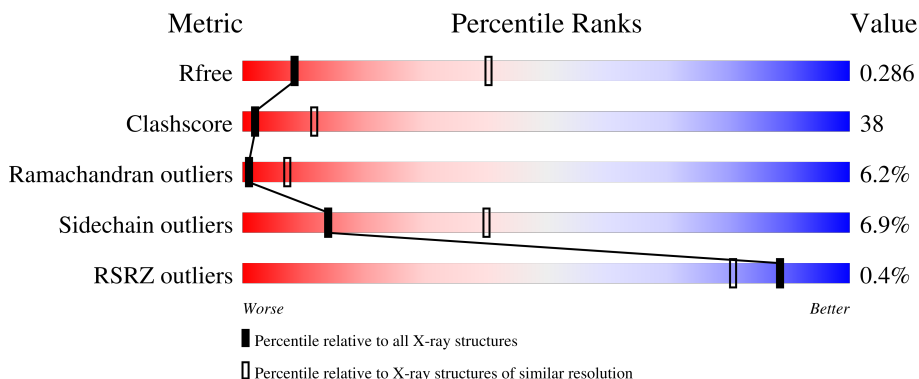
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.



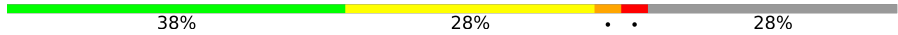


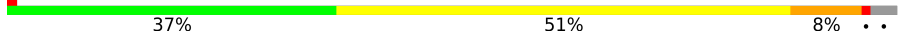
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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  $\geq 3$ , 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	452	 39% 50% 11%
1	D	452	 40% 49% 10% .
1	G	452	 36% 52% 11% .
2	B	39	 46% 21% 5% 28%
2	E	39	 33% 33% 5% 28%

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Mol	Chain	Length	Quality of chain
2	H	39	 38% 28% . . 28%
3	C	152	 36% 51% 9% . .
3	F	152	%  38% 49% 9% . .
3	I	152	%  37% 51% 8% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15021 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 NUP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	451	Total 3628	C 2323	N 587	O 707	S 11	0	0	0
1	D	447	Total 3601	C 2309	N 582	O 699	S 11	0	0	0
1	G	447	Total 3601	C 2309	N 582	O 699	S 11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	SER	CYS	conflict	UNP P40368
D	396	SER	CYS	conflict	UNP P40368
G	396	SER	CYS	conflict	UNP P40368

- Molecule 2 is a protein called Nucleoporin NUP159.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	28	Total 221	C 144	N 37	O 37	S 3	0	0	0
2	E	28	Total 221	C 144	N 37	O 37	S 3	0	0	0
2	H	28	Total 221	C 144	N 37	O 37	S 3	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1422	GLY	-	expression tag	UNP P40477
B	1423	PRO	-	expression tag	UNP P40477
B	1424	HIS	-	expression tag	UNP P40477
E	1422	GLY	-	expression tag	UNP P40477
E	1423	PRO	-	expression tag	UNP P40477

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1424	HIS	-	expression tag	UNP P40477
H	1422	GLY	-	expression tag	UNP P40477
H	1423	PRO	-	expression tag	UNP P40477
H	1424	HIS	-	expression tag	UNP P40477

- Molecule 3 is a protein called Nucleoporin 98.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	147	1176	745	202	226	3	0	0	0
3	F	147	1176	745	202	226	3	0	0	0
3	I	147	1176	745	202	226	3	0	0	0

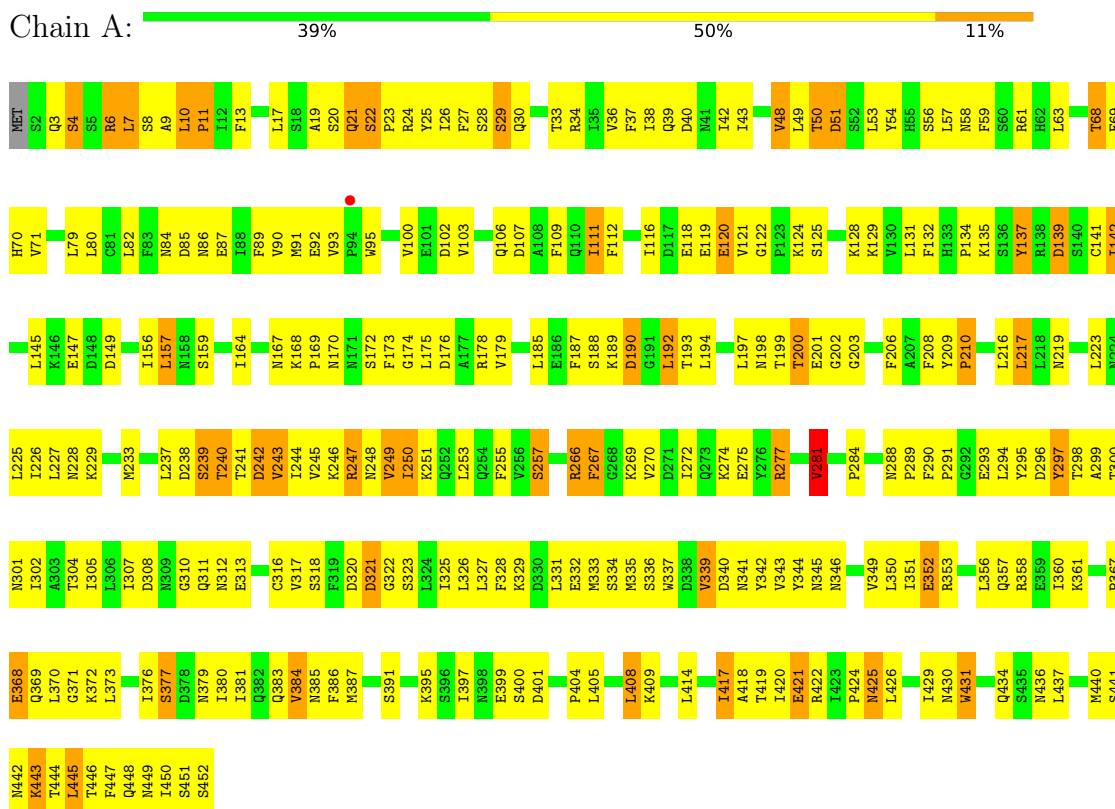
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	729	GLY	-	expression tag	UNP Q6PFD9
C	730	PRO	-	expression tag	UNP Q6PFD9
C	731	HIS	-	expression tag	UNP Q6PFD9
F	729	GLY	-	expression tag	UNP Q6PFD9
F	730	PRO	-	expression tag	UNP Q6PFD9
F	731	HIS	-	expression tag	UNP Q6PFD9
I	729	GLY	-	expression tag	UNP Q6PFD9
I	730	PRO	-	expression tag	UNP Q6PFD9
I	731	HIS	-	expression tag	UNP Q6PFD9

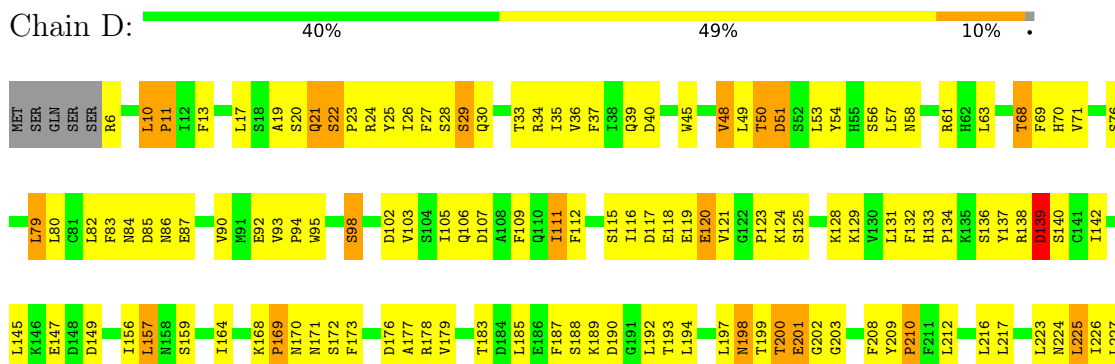
### 3 Residue-property plots

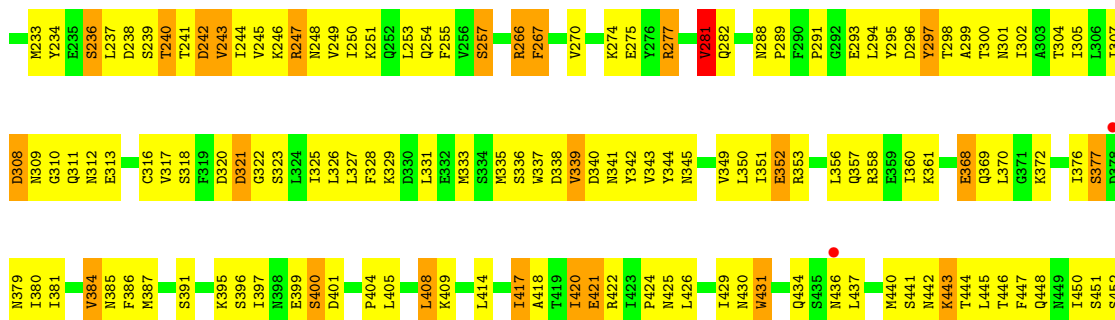
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 NUP82

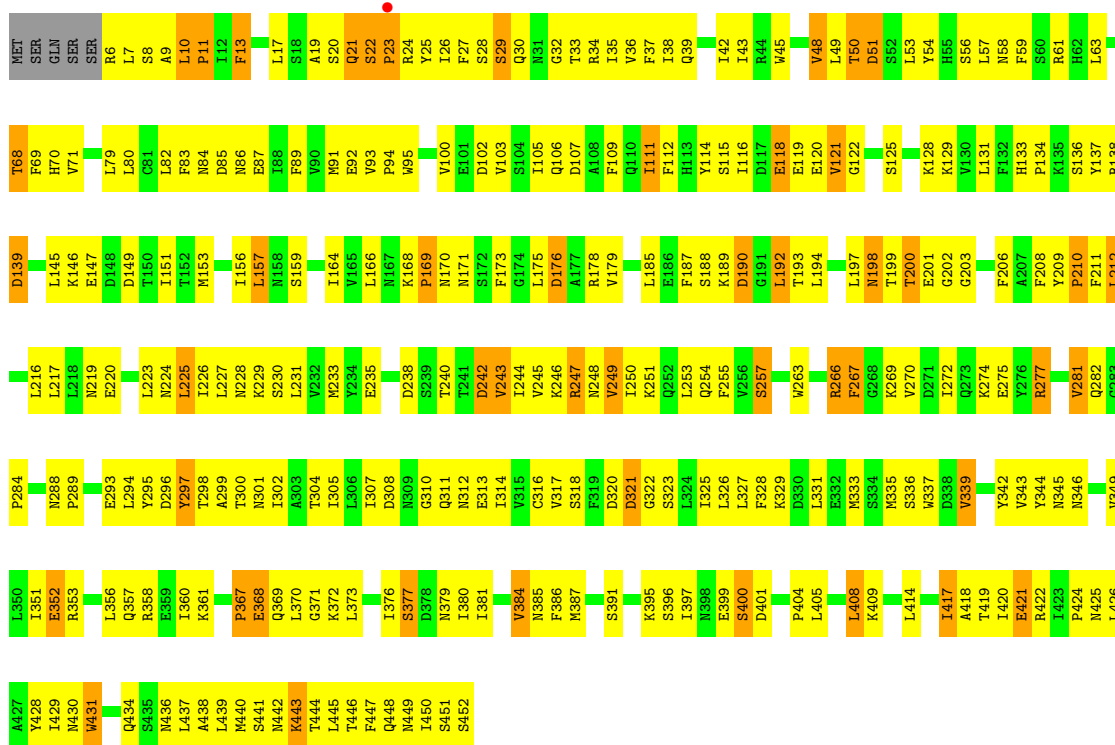


- Molecule 1: Nucleoporin NUP82





• Molecule 1: Nucleoporin NUP82



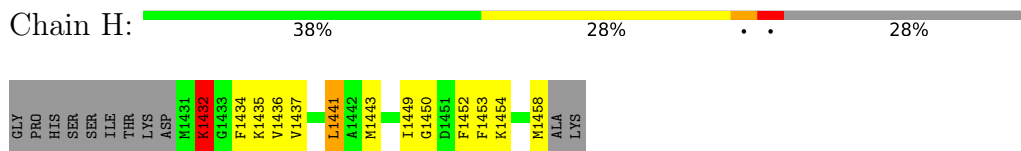
• Molecule 2: Nucleoporin NUP159



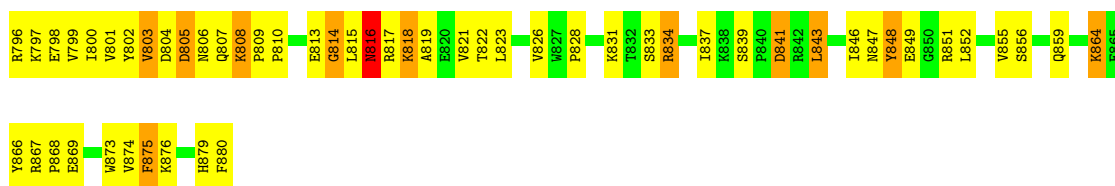
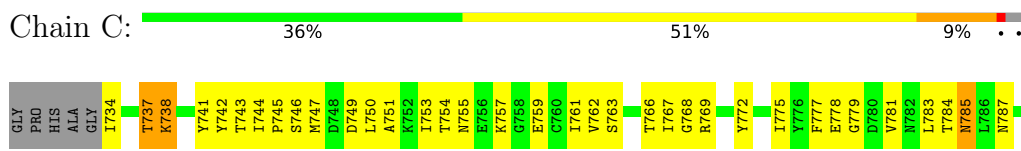
• Molecule 2: Nucleoporin NUP159



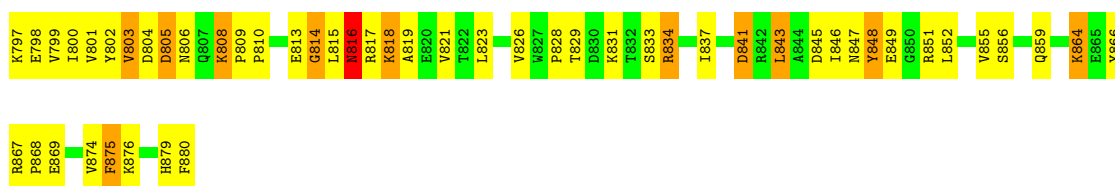
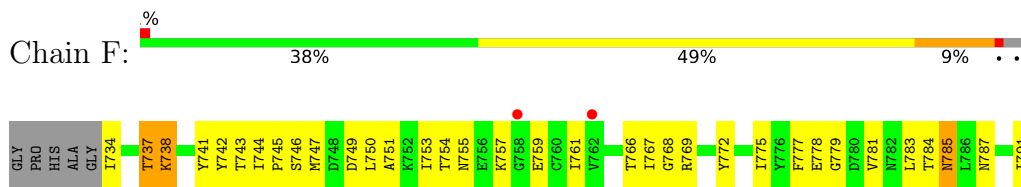
• Molecule 2: Nucleoporin NUP159



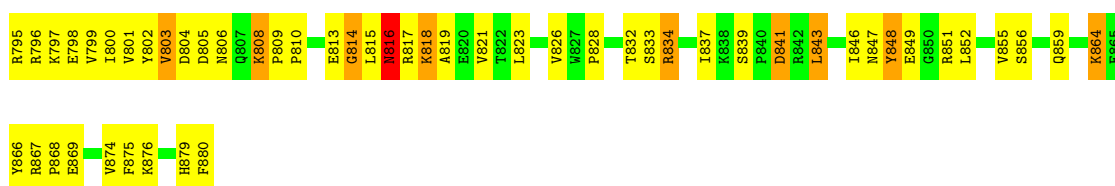
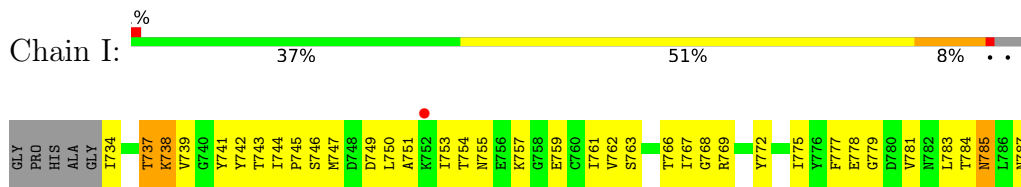
• Molecule 3: Nucleoporin 98



• Molecule 3: Nucleoporin 98



• Molecule 3: Nucleoporin 98



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.91Å 115.85Å 118.49Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.40) 92.3 (20.00-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.40Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.285 0.250 , 0.286	Depositor DCC
$R_{free}$ test set	3659 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.5	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.55	0/3701	1.03	17/5025 (0.3%)
1	D	0.65	0/3674	1.02	16/4989 (0.3%)
1	G	0.53	0/3674	1.03	14/4989 (0.3%)
2	B	0.73	0/223	0.98	0/293
2	E	0.84	0/223	0.98	1/293 (0.3%)
2	H	0.69	0/223	0.98	1/293 (0.3%)
3	C	0.42	0/1199	0.93	5/1620 (0.3%)
3	F	0.47	0/1199	0.93	5/1620 (0.3%)
3	I	0.41	0/1199	0.91	5/1620 (0.3%)
All	All	0.56	0/15315	1.00	64/20742 (0.3%)

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	SER	N-CA-C	-8.12	105.37	114.62
1	D	111	ILE	N-CA-C	8.11	118.89	110.62
1	G	190	ASP	N-CA-C	-7.96	103.58	113.38
1	G	111	ILE	N-CA-C	7.70	118.48	110.62
1	D	190	ASP	N-CA-C	-7.59	104.04	113.38

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	3628	0	3594	275	0
1	D	3601	0	3571	263	0
1	G	3601	0	3571	291	0
2	B	221	0	235	13	0
2	E	221	0	235	18	0
2	H	221	0	235	17	0
3	C	1176	0	1170	112	0
3	F	1176	0	1170	108	0
3	I	1176	0	1170	104	0
All	All	15021	0	14951	1135	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 38.

The worst 5 of 1135 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:G:37:PHE:HE1	1:G:440:MET:HE1	1.15	1.10
1:G:57:LEU:HD22	1:G:100:VAL:HG11	1.36	1.02
1:A:121:VAL:HG12	1:A:122:GLY:H	1.32	0.95
1:A:6:ARG:HB2	1:A:431:TRP:HH2	1.30	0.93
1:D:142:ILE:HG23	1:D:156:ILE:HD11	1.53	0.89

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	449/452 (99%)	358 (80%)	64 (14%)	27 (6%)	<b>1</b> <b>7</b>
1	D	445/452 (98%)	351 (79%)	65 (15%)	29 (6%)	<b>1</b> <b>6</b>
1	G	445/452 (98%)	358 (80%)	62 (14%)	25 (6%)	<b>1</b> <b>9</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	26/39 (67%)	21 (81%)	5 (19%)	0	100	100
2	E	26/39 (67%)	21 (81%)	4 (15%)	1 (4%)	2	15
2	H	26/39 (67%)	20 (77%)	6 (23%)	0	100	100
3	C	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1	5
3	F	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1	5
3	I	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1	5
All	All	1852/1929 (96%)	1459 (79%)	278 (15%)	115 (6%)	1	7

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	266	ARG
1	A	311	GLN
1	A	377	SER
3	C	738	LYS

### 5.3.2 Protein sidechains [i](#)

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	422/423 (100%)	390 (92%)	32 (8%)	12	38
1	D	418/423 (99%)	387 (93%)	31 (7%)	13	38
1	G	418/423 (99%)	387 (93%)	31 (7%)	13	38
2	B	24/33 (73%)	22 (92%)	2 (8%)	10	35
2	E	24/33 (73%)	23 (96%)	1 (4%)	26	52
2	H	24/33 (73%)	22 (92%)	2 (8%)	10	35
3	C	130/132 (98%)	123 (95%)	7 (5%)	20	47
3	F	130/132 (98%)	123 (95%)	7 (5%)	20	47
3	I	130/132 (98%)	124 (95%)	6 (5%)	24	50
All	All	1720/1764 (98%)	1601 (93%)	119 (7%)	14	40

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	251	LYS
1	G	443	LYS
1	D	443	LYS
1	G	431	TRP
3	I	864	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	113	HIS
1	G	436	ASN
3	I	862	GLN
3	I	785	ASN
1	G	346	ASN

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	451/452 (99%)	-0.25	1 (0%) 91 87	60, 104, 150, 170	0
1	D	447/452 (98%)	0.03	2 (0%) 88 81	61, 99, 145, 170	0
1	G	447/452 (98%)	-0.23	1 (0%) 91 87	63, 104, 148, 170	0
2	B	28/39 (71%)	-0.41	0 100 100	68, 90, 136, 136	0
2	E	28/39 (71%)	-0.27	0 100 100	65, 87, 127, 136	0
2	H	28/39 (71%)	-0.39	0 100 100	69, 88, 126, 137	0
3	C	147/152 (96%)	-0.14	0 100 100	95, 141, 190, 199	0
3	F	147/152 (96%)	0.06	2 (1%) 73 59	93, 140, 190, 198	0
3	I	147/152 (96%)	0.02	1 (0%) 84 73	96, 141, 190, 199	0
All	All	1870/1929 (96%)	-0.13	7 (0%) 88 81	60, 111, 169, 199	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	378	ASP	3.0
1	D	436	ASN	2.7
1	G	23	PRO	2.5
3	F	762	VAL	2.4
3	F	758	GLY	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.