



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 11:16 AM UTC

PDB ID : 2X1G / pdb_00002x1g
Title : Crystal structure of Importin13 - Mago-Y14 complex
Authors : Bono, F.; Cook, A.G.; Gruenwald, M.; Ebert, J.; Conti, E.
Deposited on : 2009-12-23
Resolution : 3.35 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

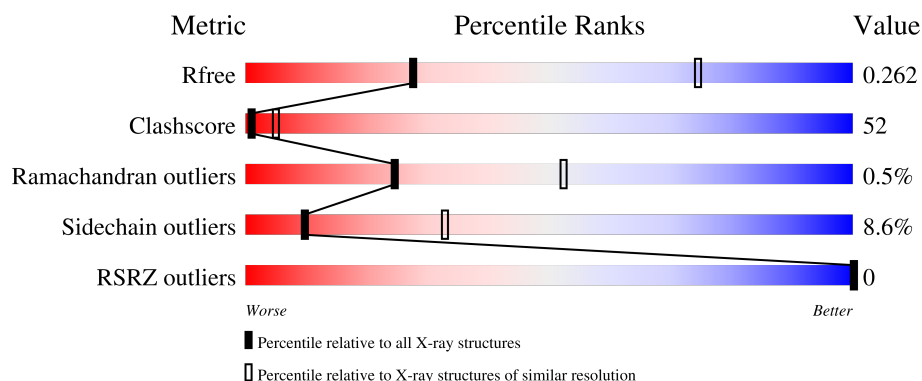
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	165	
1	C	165	
2	B	147	
2	D	147	
3	F	971	

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Mol	Chain	Length	Quality of chain
3	G	971	36% 50% 6% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16076 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 RNA-BINDING PROTEIN 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			650	415	110	122	3			
1	C	90	Total	C	N	O	S	0	0	0
			650	415	110	122	3			

- Molecule 2 is a protein called PROTEIN MAGO NASHI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	S	0	0	0
			1081	702	185	189	5			
2	D	140	Total	C	N	O	S	0	0	0
			1081	702	185	189	5			

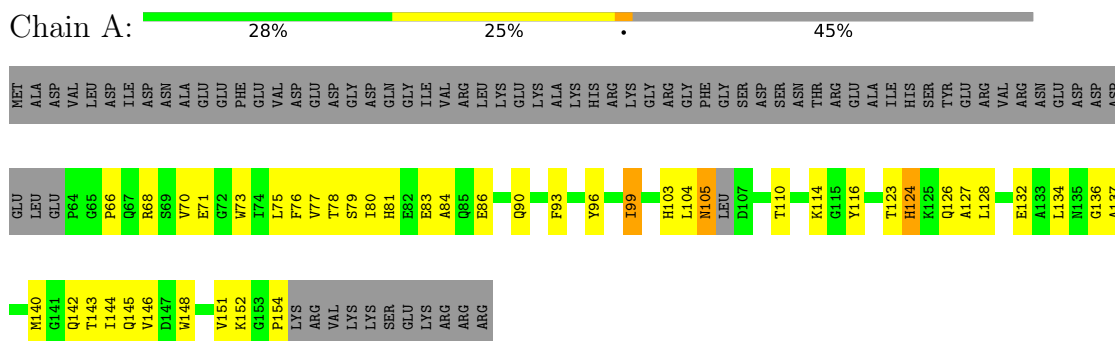
- Molecule 3 is a protein called CADMUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	896	Total	C	N	O	S	0	0	0
			6307	4043	1078	1137	49			
3	G	896	Total	C	N	O	S	0	0	0
			6307	4043	1078	1137	49			

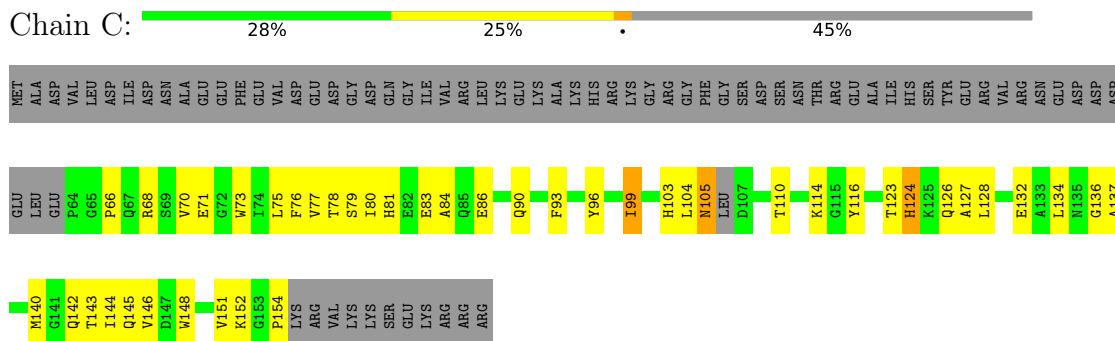
3 Residue-property plots [i](#)

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.

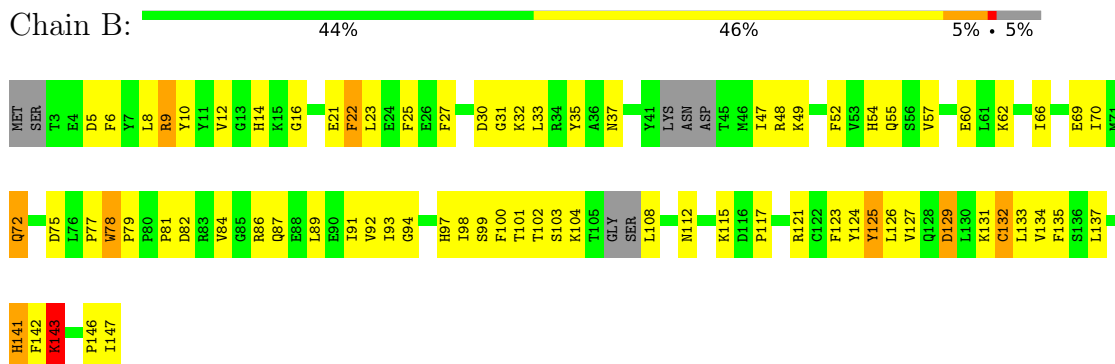
• Molecule 1: RNA-BINDING PROTEIN 8A



• Molecule 1: RNA-BINDING PROTEIN 8A

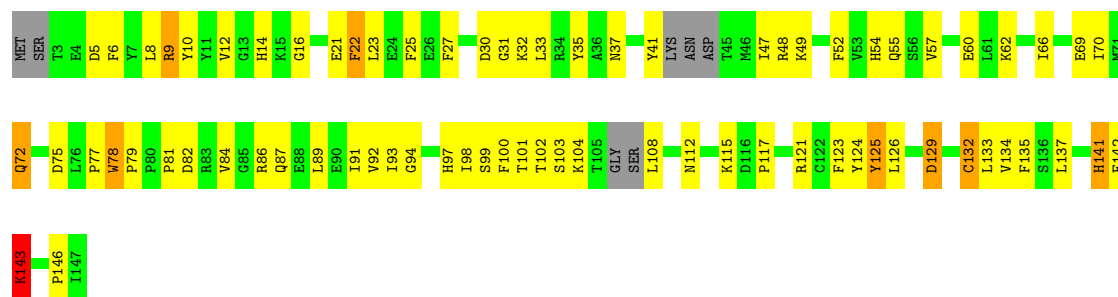


• Molecule 2: PROTEIN MAGO NASHI

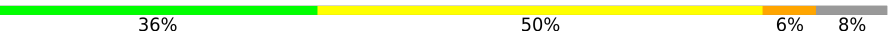


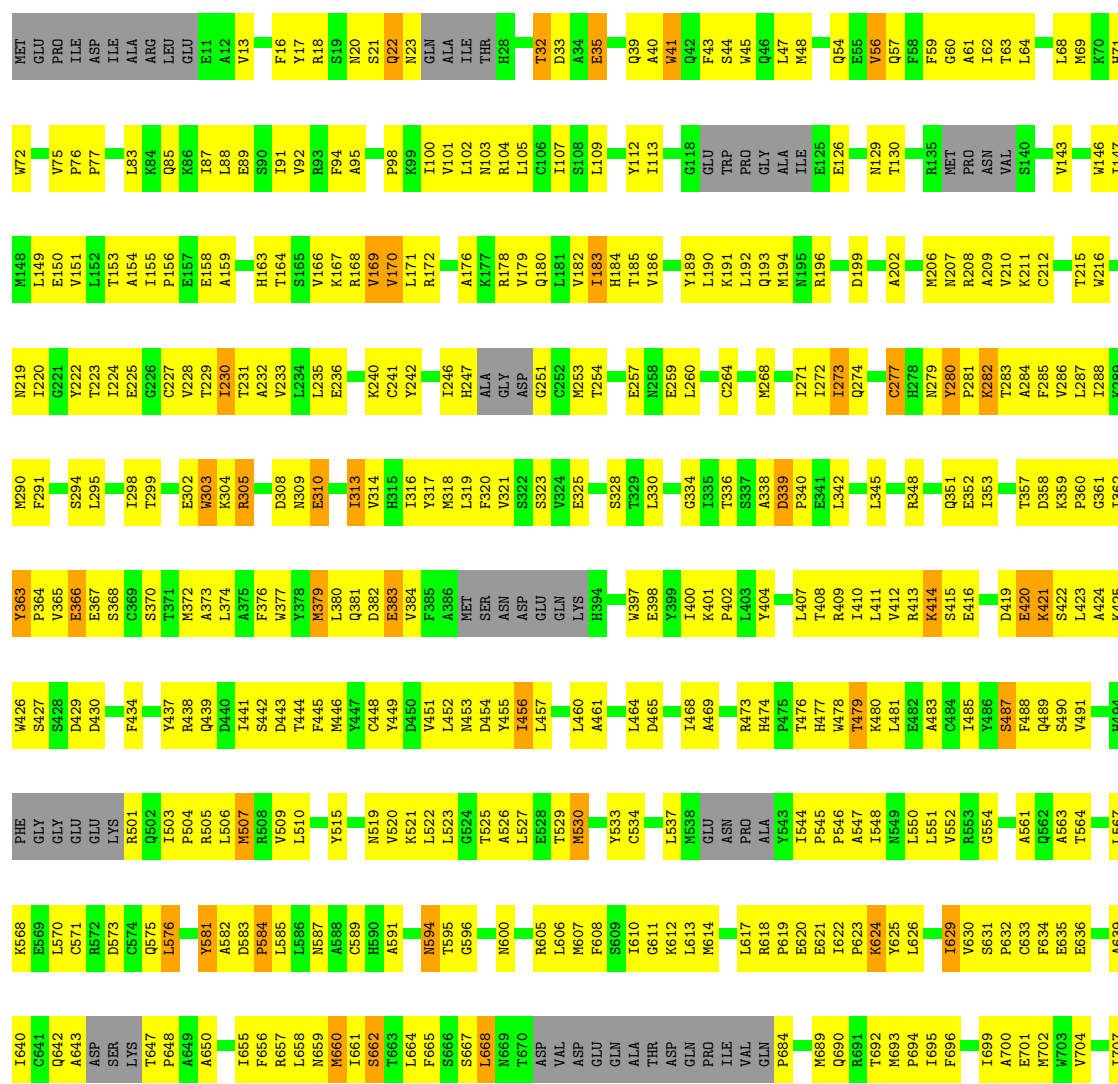
• Molecule 2: PROTEIN MAGO NASHI

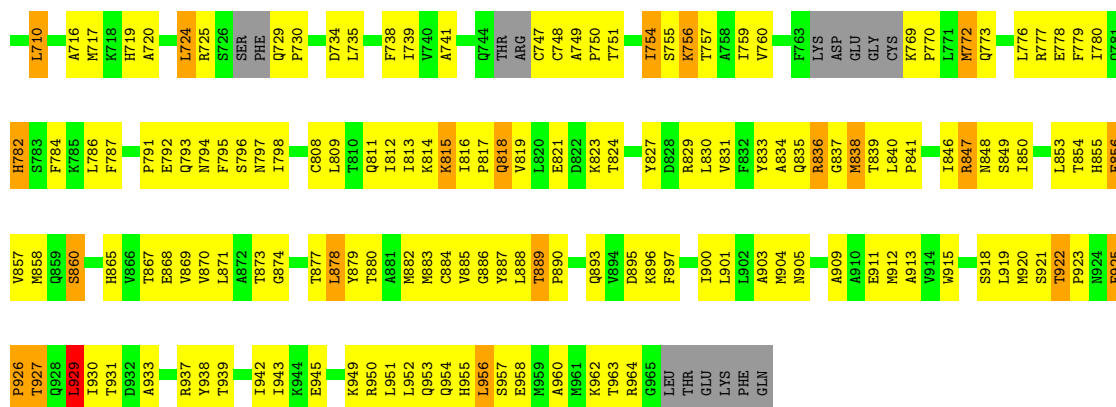
Chain D:  45% 44% 5% • 5%



• Molecule 3: CADMUS

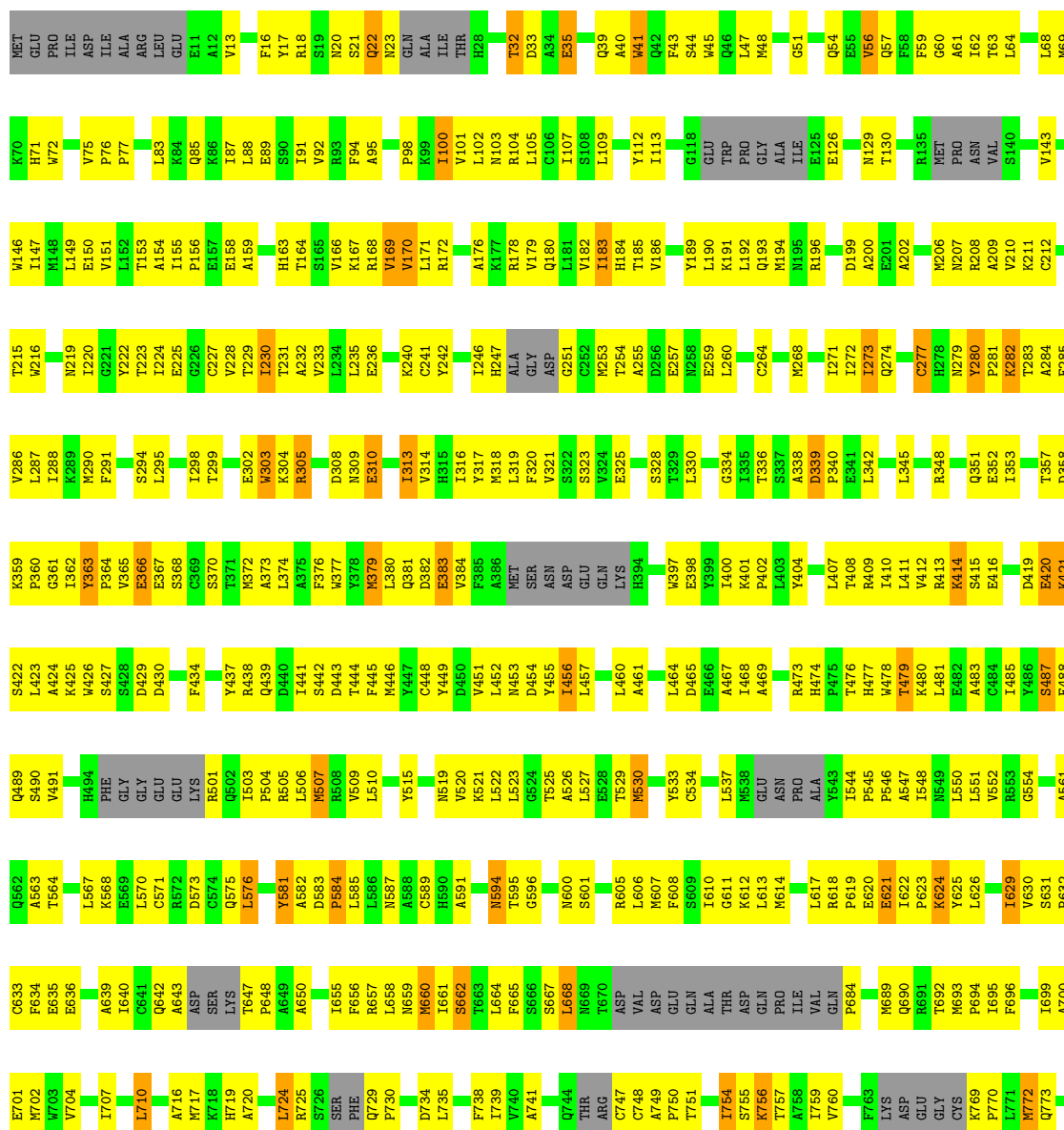
Chain F:  36% 50% 6% 8%





• Molecule 3: CADMUS

Chain G: 36% 50% 6% 8%



L776	R777	E778	F779	I780	Q781	H782	S783	F784	K785	L786	F787		P791	E792	Q793	N794	F795	S796	N797	I798		C808	L809	T810	Q811	I812	I813	K814	K815	I816	P817	Q818	V819	L820	E821	D822	K823	T824		Y827	D828	R829	L830	V831	F832	Y833	A834	Q835	R836	G837	M838	T839	L840	P841		I846	R847	N848	S849
I850		L853	T854	H855	F856	V857	M858	Q859	S860		H865	V866	T867	E868	V869	V870	L871	A872	T873	Q874		T877	L878	Y879	T880	A881	M882	M883	C884	V885	G886	Y887	L888	T889	P890		Q893	V894	D895	K896	F897		I900	L901	L902	A903	M904	N905		A909	A910	E911	M912	A913	V914	W915		S918	L919
M920	S921	T922	P923	N924	F925	P926	T927	Q928	L929		T930	D932	A933		R937	Y938	T939		I942	I943	K944	E945		K949	R950	L951	L952	Q953	Q954	H955	L956	S957	E958	M959	A960	M961	K962	T963	R964	G965	LEU	THR	GLU	LYS	PHE	GLN													

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.57Å 100.79Å 93.92Å 89.83° 110.18° 90.63°	Depositor
Resolution (Å)	50.00 – 3.35 50.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-3.35) 93.2 (50.00-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.267 , 0.289 0.259 , 0.262	Depositor DCC
R_{free} test set	2376 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 135.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.388 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16076	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	0.43	0/665	0.92	1/907 (0.1%)
1	C	0.43	0/665	0.92	1/907 (0.1%)
2	B	0.42	0/1108	0.95	4/1499 (0.3%)
2	D	0.42	0/1108	0.95	4/1499 (0.3%)
3	F	0.51	2/6416 (0.0%)	1.07	32/8773 (0.4%)
3	G	0.51	2/6416 (0.0%)	1.07	32/8773 (0.4%)
All	All	0.50	4/16378 (0.0%)	1.04	74/22358 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	782	HIS	CB-CG	-5.95	1.41	1.50
3	G	782	HIS	CB-CG	-5.93	1.41	1.50
3	F	702	MET	SD-CE	5.92	1.94	1.79
3	G	702	MET	SD-CE	5.92	1.94	1.79

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	926	PRO	N-CA-C	-11.65	97.92	113.65
3	G	926	PRO	N-CA-C	-11.63	97.95	113.65
3	G	21	SER	N-CA-C	9.57	121.40	110.97
3	F	21	SER	N-CA-C	9.53	121.36	110.97
3	F	421	LYS	N-CA-C	-8.91	101.52	111.14

There are no chirality outliers.

There are no planarity outliers.

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	650	0	561	48	0
1	C	650	0	561	51	0
2	B	1081	0	987	97	0
2	D	1081	0	987	92	1
3	F	6307	0	5647	670	1
3	G	6307	0	5647	669	0
All	All	16076	0	14390	1572	1

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 52.

The worst 5 of 1572 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)
3:G:224:ILE:HD11	3:G:277:CYS:HB3	1.19	1.17
3:F:760:VAL:HA	3:F:816:ILE:CD1	1.74	1.17
3:G:274:GLN:HB2	3:G:277:CYS:SG	1.85	1.16
3:G:760:VAL:HA	3:G:816:ILE:CD1	1.74	1.15
3:F:274:GLN:HB2	3:F:277:CYS:SG	1.85	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:TYR:O	3:F:259:GLU:OE1[1_545]	2.11	0.09

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	86/165 (52%)	78 (91%)	8 (9%)	0	100	100
1	C	86/165 (52%)	78 (91%)	8 (9%)	0	100	100
2	B	134/147 (91%)	120 (90%)	14 (10%)	0	100	100
2	D	134/147 (91%)	120 (90%)	14 (10%)	0	100	100
3	F	870/971 (90%)	783 (90%)	82 (9%)	5 (1%)	21	49
3	G	870/971 (90%)	782 (90%)	83 (10%)	5 (1%)	21	49
All	All	2180/2566 (85%)	1961 (90%)	209 (10%)	10 (0%)	24	52

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	874	GLY
3	G	874	GLY
3	F	818	GLN
3	G	818	GLN
3	F	584	PRO

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	56/141 (40%)	52 (93%)	4 (7%)	13	39
1	C	56/141 (40%)	52 (93%)	4 (7%)	13	39
2	B	103/136 (76%)	95 (92%)	8 (8%)	11	37
2	D	103/136 (76%)	95 (92%)	8 (8%)	11	37
3	F	549/871 (63%)	500 (91%)	49 (9%)	9	31
3	G	549/871 (63%)	500 (91%)	49 (9%)	9	31
All	All	1416/2296 (62%)	1294 (91%)	122 (9%)	10	33

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	710	LEU

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Mol	Chain	Res	Type
3	G	836	ARG
3	F	956	LEU
3	G	772	MET
3	G	927	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	307	ASN
3	G	659	ASN
3	F	659	ASN
3	G	594	ASN
3	G	893	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	90/165 (54%)	-1.38	0 100 100	45, 86, 142, 169	0
1	C	90/165 (54%)	-1.38	0 100 100	45, 86, 142, 169	0
2	B	140/147 (95%)	-1.33	0 100 100	33, 87, 168, 187	0
2	D	140/147 (95%)	-1.35	0 100 100	33, 87, 168, 187	0
3	F	896/971 (92%)	-1.32	0 100 100	38, 97, 157, 197	0
3	G	896/971 (92%)	-1.31	0 100 100	38, 97, 157, 197	0
All	All	2252/2566 (87%)	-1.32	0 100 100	33, 95, 157, 197	0

There are no RSRZ outliers to report.

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.