



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 01:25 PM EST

PDB ID : 3JRO
Title : NUP84-NUP145C-SEC13 edge element of the NPC lattice
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Deposited on : 2009-09-08
Resolution : 4.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

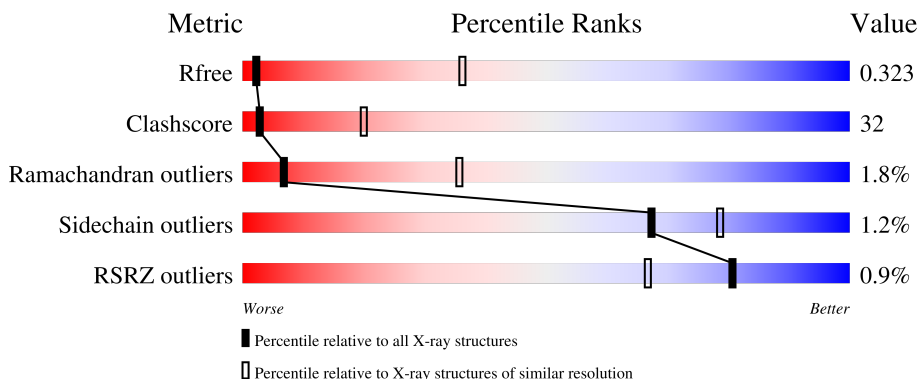
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


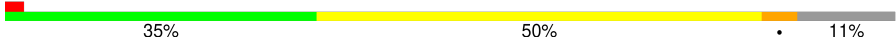
The reported resolution of this entry is 4.00 Å.

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}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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	753	
2	C	426	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8671 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 Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	Se	0	0	0
			5623	3598	943	1068	9	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1100	GLY	-	linker	UNP P49687
A	1101	GLY	-	linker	UNP P49687
A	1102	GLY	-	linker	UNP P49687
A	1103	GLY	-	linker	UNP P49687
A	1104	SER	-	linker	UNP P49687
A	1105	GLY	-	linker	UNP P49687
A	1106	GLY	-	linker	UNP P49687
A	1107	GLY	-	linker	UNP P49687
A	1108	GLY	-	linker	UNP P49687

- Molecule 2 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	379	Total	C	N	O	S	Se	0	0	0
			3048	1949	504	584	4	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P52891
C	0	SER	-	expression tag	UNP P52891

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.

- Chain A: 54% ● 7%

Residue	L1519	L1520	N1524	L1528	L1532	A1541	L1544	K1545	Y1548	L1553	SER	GLU
L1519	D1335	Y1426	L1336	A1259	L1160	L1161	E294	K1263	S1169	GLN	GLY	GLU
L1520	A1427	L1337	A1337	L1260	L1260	L1261	E294	K1263	G1170	GLY	GLY	GLU
N1524	A1428	A1338	A1338	L1261	L1261	L1262	E294	K1263	V1171	GLY	GLY	GLU
L1528	T1432	Q1340	L1341	R1265	R1265	R1266	E294	K1263	L1176	SER	SER	A108
L1532	L1435	W1344	Y1436	R1268	R1268	R1269	E294	K1263	P1177	GLY	GLY	A109
A1541	K1437	K1437	K1437	R1269	R1269	R1270	E294	K1263	T1178	GLY	GLY	H110
L1544	E1438	Q1439	S1350	I1273	I1273	I1274	E294	K1263	Q1181	GLY	GLY	A111
K1545	V1439	I1351	D1352	I1277	I1277	I1278	E294	K1263	R1182	GLY	GLY	L112
Y1548	R1442	K1353	K1353	I1281	I1281	I1282	E294	K1263	F1186	GLY	GLY	D114
L1553	Q1449	I1355	I1355	I1285	I1285	I1286	E294	K1263	L1191	GLY	GLY	A115
SER	L1454	P1366	P1366	I1292	I1292	I1293	E294	K1263	I1196	GLY	GLY	L116
GLU	L1455	F1367	F1367	I1294	I1294	I1295	E294	K1263	E1196	GLY	GLY	S126
	L1458	F1371	F1371	I1298	I1298	I1299	E294	K1263	V1198	GLY	GLY	V127
	F1460	K1374	K1374	I1300	I1300	I1301	E294	K1263	L1198	GLY	GLY	V128
	T1463	E1377	E1377	N1302	N1302	N1303	E294	K1263	Y1208	GLY	GLY	E129
R1464	F1465	W1382	W1382	D1303	D1303	D1304	E294	K1263	P1209	GLY	GLY	T140
F1466	F1466	L1383	L1383	Q1210	Q1210	Q1211	E294	K1263	L1209	GLY	GLY	S126
T1470	T1470	L1384	L1384	I1211	I1211	I1212	E294	K1263	E1211	GLY	GLY	V127
F1484	F1484	N1387	N1387	R1305	R1305	R1306	E294	K1263	S1214	GLY	GLY	V128
L1487	L1487	L1388	L1388	S1214	S1214	S1215	E294	K1263	E1214	GLY	GLY	E129
H1488	H1488	T1389	T1389	K1219	K1219	K1220	E294	K1263	L1219	GLY	GLY	T140
G1489	G1489	L1390	L1390	L1222	L1222	L1223	E294	K1263	L1222	GLY	GLY	S126
H1490	H1490	C1391	C1391	L1234	L1234	L1235	E294	K1263	L1234	GLY	GLY	H144
S1491	S1491	Y1392	Y1392	L1237	L1237	L1238	E294	K1263	L1237	GLY	GLY	S126
L1492	L1492	G1393	G1393	S1238	S1238	S1239	E294	K1263	E1238	GLY	GLY	V148
		Q1394	Q1394	L1240	L1240	L1241	E294	K1263	I1240	GLY	GLY	A151
S1495	S1495	L1395	L1395	F1242	F1242	F1243	E294	K1263	I1241	GLY	GLY	S152
C1496	C1496	D1396	D1396	D1243	D1243	D1244	E294	K1263	F1242	GLY	GLY	S153
F1497	F1497	L1400	L1400	L1244	L1244	L1245	E294	K1263	E1243	GLY	GLY	R65
L1498	L1498	E1401	E1401	V1245	V1245	V1246	E294	K1263	F1244	GLY	GLY	F66
		S1402	S1402	P1248	P1248	P1249	E294	K1263	E1244	GLY	GLY	T157
A1504	A1504	L1403	L1403	L1322	L1322	L1323	E294	K1263	L1322	GLY	GLY	I157
E1505	E1505	V1404	V1404	L1324	L1324	L1325	E294	K1				

- Chain C:  2% 35% 50% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 170.47Å 270.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.89 – 4.00 49.89 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.89-4.00) 99.8 (49.89-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.282 , 0.329 0.276 , 0.323	Depositor DCC
R_{free} test set	1586 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å ²)	133.7	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 144.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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	0.24	0/5744	0.41	0/7776
2	C	0.28	0/3101	0.49	0/4202
All	All	0.25	0/8845	0.44	0/11978

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

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	5623	0	5577	286	0
2	C	3048	0	3033	306	0
All	All	8671	0	8610	555	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 32.

The worst 5 of 555 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)
2:C:104:LEU:HA	2:C:219:LEU:HD12	1.19	1.09
2:C:215:ILE:HG21	2:C:267:LEU:HD13	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:HIS:HB2	2:C:160:PHE:HB2	1.44	0.99
2:C:412:LEU:HB3	2:C:416:TYR:HE2	1.32	0.94
1:A:1251:THR:H	1:A:1257:LYS:HE2	1.35	0.91

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	695/753 (92%)	608 (88%)	78 (11%)	9 (1%)	10	42
2	C	373/426 (88%)	297 (80%)	66 (18%)	10 (3%)	4	29
All	All	1068/1179 (91%)	905 (85%)	144 (14%)	19 (2%)	7	36

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	218	TYR
2	C	281	ASP
2	C	55	ASN
2	C	171	VAL
2	C	222	VAL

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	621/655 (95%)	618 (100%)	3 (0%)	86	89
2	C	345/384 (90%)	336 (97%)	9 (3%)	41	61
All	All	966/1039 (93%)	954 (99%)	12 (1%)	67	78

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	249	SER
2	C	280	SER
2	C	395	CYS
2	C	301	TYR
2	C	58	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	360	HIS
2	C	300	ASN
2	C	240	HIS
2	C	234	GLN
2	C	273	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	696/753 (92%)	-0.21	1 (0%) 92 89	159, 188, 244, 325	0
2	C	372/426 (87%)	0.15	9 (2%) 59 45	134, 171, 248, 370	0
All	All	1068/1179 (90%)	-0.09	10 (0%) 81 67	134, 183, 246, 370	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	287	HIS	3.4
2	C	416	TYR	3.1
2	C	289	HIS	3.1
2	C	397	ASP	2.7
1	A	1133	ILE	2.4

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 monosaccharides 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.