wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 01:38 PM JST

PDB ID	:	7V1M
Title	:	Structural basis for the co-chaperone relationship of sNASP and ASF1b
Authors	:	Bao, H.; Huang, H.
Deposited on	:	2021-08-04
Resolution	:	2.83 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 (i) symbol.

The types of validation reports are described at
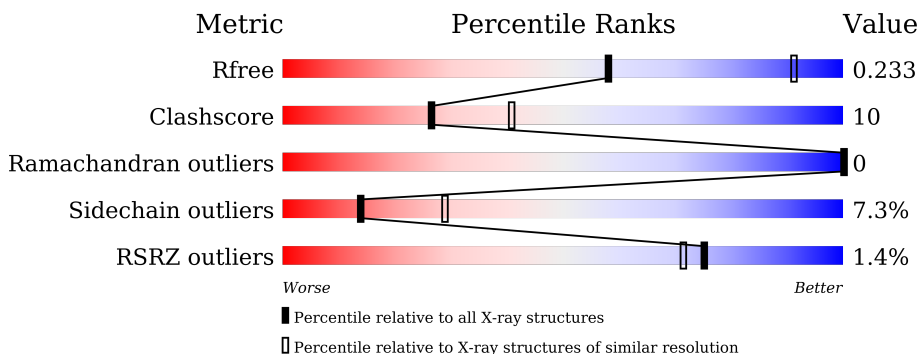http://www.wwpdb.org/validation/2017/FAQs#types.

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 2.83 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.
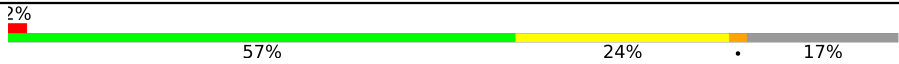
Metric	Percentile Ranks	Value
Rfree		0.233
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		7.3%
RSRZ outliers		1.4%

Worse ... *Better*

∎ Percentile relative to all X-ray structures

⧄ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 <=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	135	42% 13% • 44%
1	B	135	% 42% 21% • 36%
2	C	102	60% 19% 22%
2	E	102	% 59% 16% • 24%
3	D	158	71% 27% •
3	F	158	71% 24% • •

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
4	G	235	2% · · · 57% · · · 24% · 17%
4	H	235	3% · · · 57% · · · 27% · 15%

2 Entity composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7966 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 Histone H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	86	Total	C	N	O	S	0	0	0
			679	430	126	121	2			
1	A	75	Total	C	N	O	S	0	0	0
			583	370	110	101	2			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	S	0	0	0
			620	393	118	108	1			
2	E	78	Total	C	N	O	S	0	0	0
			605	383	115	106	1			

- Molecule 3 is a protein called Histone chaperone ASF1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	154	Total	C	N	O	S	0	0	0
			1230	790	203	232	5			
3	F	154	Total	C	N	O	S	0	0	0
			1220	784	201	230	5			

- Molecule 4 is a protein called Isoform 2 of Nuclear autoantigenic sperm protein.

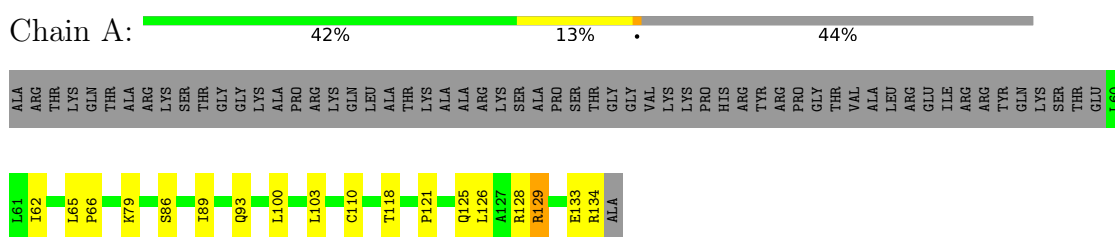| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	195	Total	C	N	O	S	0	0	0
			1480	930	243	303	4			
4	H	200	Total	C	N	O	S	0	0	0
			1549	979	254	311	5			

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.
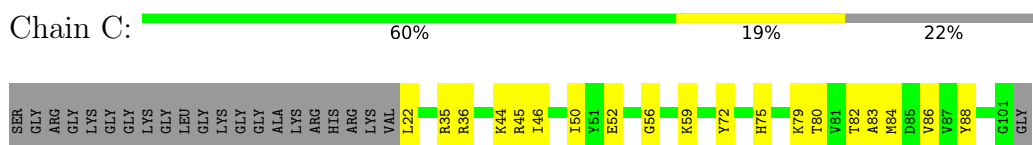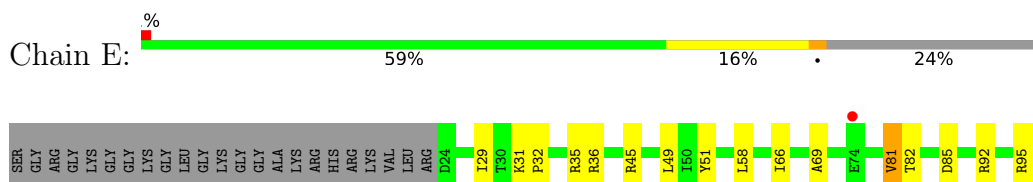
- Molecule 1: Histone H3.3

Chain B:

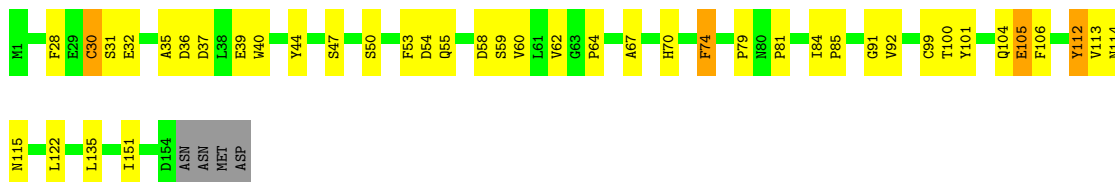- Molecule 1: Histone H3.3

Chain A:

- Molecule 2: Histone H4

Chain C:

- Molecule 2: Histone H4

Chain E:

- Molecule 3: Histone chaperone ASF1B

Chain D:

M1 A2 K3 A10 N14 F22 E25 I26 E29 C30 S31 E32 A33 D36 D37 L38 E39 W40 K41 S47 A48 E49 S50 E51 G63 A67 G68 R69 F72 V73 F74 P79 T87 H102 E105 F106 I107 R108 V109 Y112 N115 E116 Y117

L135 Q136 I139 L140 A141 S142 V146 H150 I151 N152 W153 D154 ASN ASN MET ASP

• Molecule 3: Histone chaperone ASF1B

Chain F:

71% 24% • •

M1 F28 E29 C30 S31 E32 A35 D36 D37 L38 E39 W40 Y44 S47 S50 F53 D54 Q55 D58 S59 V60 L61 V62 G63 P64 A67 H70 F74 P79 N80 P81 I84 P85 G91 V92 C99 T100 Y101 Q104 E105 F106 Y112 V113 N114

N115 L122 L135 I151 D154 ASN ASN MET ASP

• Molecule 4: Isoform 2 of Nuclear autoantigenic sperm protein

Chain G:

2%

57% 24% • 17%

SER ALA ASP LYS VAL GLU SER LEU ASP VAL D40 S41 K45 L54 D58 I59 P60 A61 N64 Q67 K75 K76 Y77 A81 N82 E83 C84 G85 E86 E97 R100 LEU GLU ASN LYS SER LEU GLN GLU ASN GLU GLU GLU E172 I173 E177 W180 L185

A186 K187 I188 I189 F190 K191 R192 A198 Y201 A202 A203 H206 L207 K208 L209 G210 E211 V212 S213 A222 V223 E224 E225 F226 L232 Y236 L243 L244 A245 E246 T247 H248 Y255 N258 S259 Q260 E263 Q267 F268 S271 V274 M279 L282 ASN GLU

GLN VAL LYS GLU ALA GLU GLY SER SER ALA GLU TYR LYS K298 E299 I300 E301 E302 L303 L307 P308 S320 GLN ARG SER

• Molecule 4: Isoform 2 of Nuclear autoantigenic sperm protein

Chain H:

3%

57% 27% • 15%

SER ALA ASP LYS VAL GLU SER LEU D38 L46 Q51 K52 H53 L54 V55 M56 F66 Q67 E68 A69 A70 S71 L72 L73 G74 K75 K76 C84 F88 F89 F90 L95 L96 A99 R100 LEU GLU ASN LYS SER LEU GLN GLU ASN GLU E170 I173 G174 N175 L176 E177 L178

A179 M182 L183 D184 I188 I189 F190 A198 Y201 A202 H206 L207 S213 S216 E217 N218 Y219 V220 Q221 A222 V223 E224 E225 F226 Q227 S228 C229 L230 N231 L232 Q235 H240 T247 H248 L251 Y257 I272 E273 V274 I275 E276 M279 A280 N283 E284

GLN VAL LYS GLU ALA GLU GLY SER SER ALA GLU TYR LYS LYS E299 I300 E301 E305 L306 E309 I310 K313 E319 S320 GLN ARG SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.95Å 71.90Å 93.43Å 70.67° 70.64° 83.61°	Depositor
Resolution (Å)	35.59 – 2.83 35.59 – 2.83	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.59-2.83) 94.8 (35.59-2.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.202 , 0.240 0.199 , 0.233	Depositor DCC
R_{free} test set	1832 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	72.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -k,-h,-l	Depositor
Outliers	0 of 37598 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7966	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.64	0/590	0.75	0/790
1	B	0.51	0/687	0.69	0/923
2	C	0.53	0/627	0.72	0/842
2	E	0.58	0/612	0.73	0/820
3	D	0.63	0/1265	0.68	0/1729
3	F	0.61	0/1255	0.70	0/1715
4	G	0.58	0/1500	0.61	0/2019
4	H	0.57	0/1570	0.62	0/2112
All	All	0.59	0/8106	0.67	0/10950

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	583	0	586	16	0
1	B	679	0	686	18	0
2	C	620	0	638	9	0
2	E	605	0	615	12	0
3	D	1230	0	1186	24	0
3	F	1220	0	1157	25	0
4	G	1480	0	1345	30	0
4	H	1549	0	1462	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7966	0	7675	161	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 10.

The worst 5 of 161 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)
4:H:232:LEU:O	4:H:235:GLN:HB2	1.88	0.74
1:B:51:ILE:HD12	4:H:184:ASP:HB3	1.75	0.68
1:B:113:HIS:NE2	3:D:140:LEU:HD21	2.12	0.64
4:H:84:CYS:HB3	4:H:88:PHE:CE1	2.34	0.63
2:C:72:TYR:HA	2:C:75:HIS:HB3	1.82	0.61

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	73/135 (54%)	68 (93%)	5 (7%)	0	100	100
1	B	84/135 (62%)	76 (90%)	8 (10%)	0	100	100
2	C	78/102 (76%)	78 (100%)	0	0	100	100
2	E	76/102 (74%)	73 (96%)	3 (4%)	0	100	100
3	D	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
3	F	152/158 (96%)	144 (95%)	8 (5%)	0	100	100
4	G	189/235 (80%)	182 (96%)	7 (4%)	0	100	100
4	H	194/235 (83%)	185 (95%)	9 (5%)	0	100	100
All	All	998/1260 (79%)	952 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	56/109 (51%)	51 (91%)	5 (9%)	9	20
1	B	67/109 (62%)	62 (92%)	5 (8%)	13	28
2	C	61/78 (78%)	56 (92%)	5 (8%)	11	24
2	E	58/78 (74%)	52 (90%)	6 (10%)	7	15
3	D	138/142 (97%)	129 (94%)	9 (6%)	17	33
3	F	133/142 (94%)	128 (96%)	5 (4%)	33	59
4	G	138/197 (70%)	123 (89%)	15 (11%)	6	13
4	H	152/197 (77%)	143 (94%)	9 (6%)	19	37
All	All	803/1052 (76%)	744 (93%)	59 (7%)	14	29

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	92	ARG
4	H	218	ASN
4	G	41	SER
4	H	216	SER
4	G	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	55	GLN
3	F	134	GLN
3	F	136	GLN
4	H	51	GLN
4	H	175	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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	75/135 (55%)	0.06	0	100	100	42, 68, 100, 134	0
1	B	86/135 (63%)	0.10	1 (1%)	79	76	44, 71, 100, 120	0
2	C	80/102 (78%)	-0.07	0	100	100	46, 68, 112, 126	0
2	E	78/102 (76%)	0.12	1 (1%)	77	74	45, 66, 118, 124	0
3	D	154/158 (97%)	0.00	0	100	100	41, 60, 87, 103	0
3	F	154/158 (97%)	-0.01	0	100	100	37, 58, 83, 116	0
4	G	195/235 (82%)	0.06	5 (2%)	56	51	55, 88, 119, 141	0
4	H	200/235 (85%)	0.15	7 (3%)	44	36	57, 82, 114, 127	0
All	All	1022/1260 (81%)	0.06	14 (1%)	75	71	37, 73, 111, 141	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	282	LEU	4.5
4	G	185	LEU	4.0
4	H	305	GLU	3.6
4	H	89	PHE	3.5
4	H	240	HIS	3.1

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides 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.