



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:56 pm BST

PDB ID : 3SBG
Title : Crystal structure of a Prp8 C-terminal fragment
Authors : Weber, G.; Santos, K.; Holton, N.; Wahl, M.C.
Deposited on : 2011-06-04
Resolution : 3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

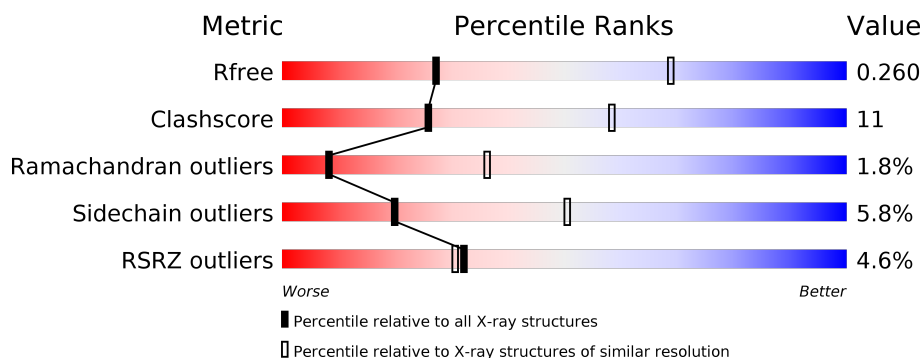
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 on 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	565	<div> <div>4%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3983 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3983	2561	656	751	15			

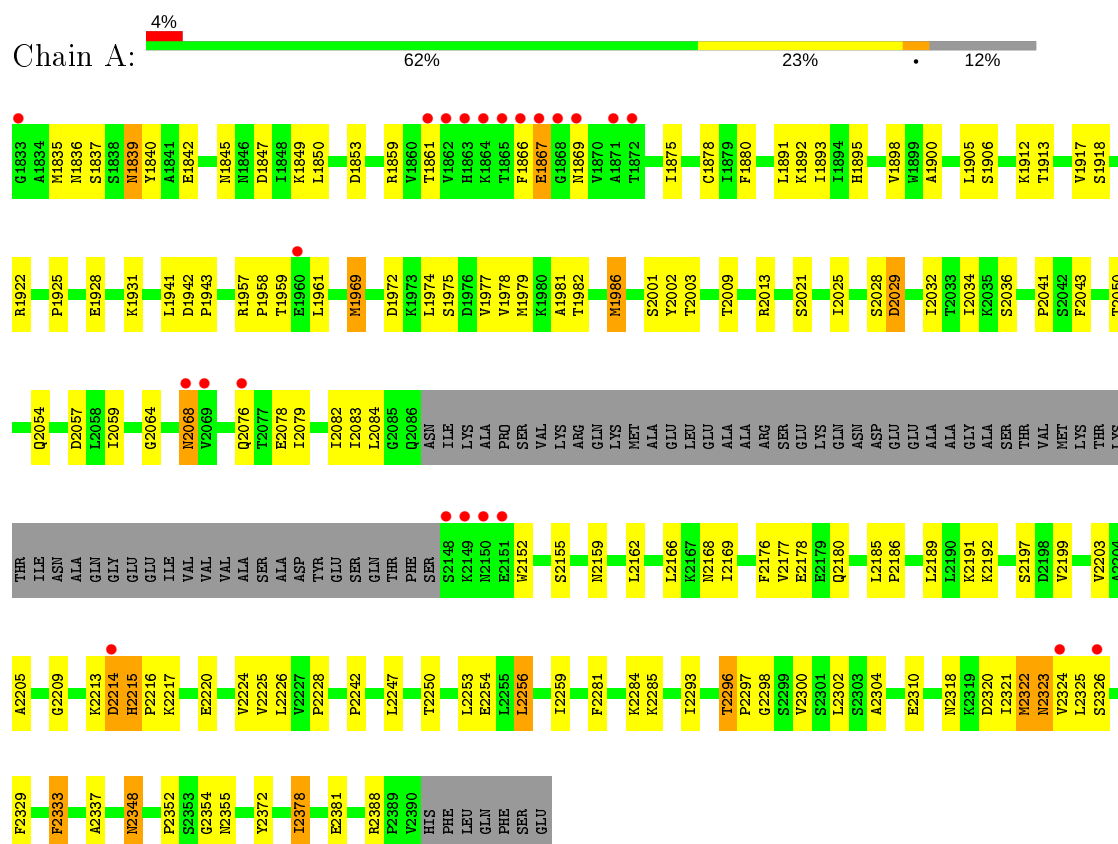
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	EXPRESSION TAG	UNP P33334
A	1834	ALA	-	EXPRESSION TAG	UNP P33334
A	1835	MET	-	EXPRESSION TAG	UNP P33334

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Pre-mRNA-splicing factor 8



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.79Å 73.60Å 72.88Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	27.08 – 3.28 27.11 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.8 (27.08-3.28) 98.8 (27.11-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.264 0.216 , 0.260	Depositor DCC
R_{free} test set	585 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3983	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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	0.22	0/4070	0.41	0/5521

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 [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	3983	0	3994	84	0
All	All	3983	0	3994	84	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 11.

All (84) 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:A:2259:ILE:HD11	1:A:2293:ILE:HD11	1.68	0.75
1:A:2076:GLN:HE21	1:A:2076:GLN:HA	1.55	0.71
1:A:1969:MET:HE1	1:A:1978:VAL:HG21	1.73	0.70
1:A:2152:TRP:CH2	1:A:2388:ARG:HB3	2.29	0.68
1:A:2321:ILE:HD12	1:A:2322:MET:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2013:ARG:HG2	1:A:2059:ILE:HD13	1.77	0.65
1:A:2321:ILE:HD12	1:A:2322:MET:N	2.16	0.61
1:A:1912:LYS:HD3	1:A:1912:LYS:O	2.01	0.61
1:A:1892:LYS:HD3	1:A:1986:MET:HG2	1.82	0.61
1:A:1853:ASP:HB3	1:A:1880:PHE:HB3	1.82	0.61
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	1.82	0.60
1:A:2028:SER:O	1:A:2029:ASP:C	2.40	0.60
1:A:1835:MET:HB2	1:A:1957:ARG:HH22	1.67	0.59
1:A:2296:THR:OG1	1:A:2297:PRO:HD2	2.03	0.58
1:A:2214:ASP:O	1:A:2215:HIS:HB2	2.03	0.58
1:A:2281:PHE:HB3	1:A:2285:LYS:O	2.04	0.58
1:A:2177:VAL:H	1:A:2180:GLN:HE21	1.51	0.58
1:A:2159:ASN:ND2	1:A:2199:VAL:HG13	2.19	0.58
1:A:2185:LEU:HD12	1:A:2186:PRO:HD2	1.86	0.58
1:A:2197:SER:HA	1:A:2203:VAL:HG21	1.84	0.58
1:A:1835:MET:HB2	1:A:1957:ARG:NH2	2.19	0.57
1:A:2189:LEU:HD13	1:A:2224:VAL:HG23	1.86	0.57
1:A:1918:SER:O	1:A:1922:ARG:HG3	2.04	0.57
1:A:1861:THR:HG23	1:A:1875:ILE:HD13	1.87	0.57
1:A:1835:MET:HA	1:A:1839:ASN:HD21	1.70	0.56
1:A:2192:LYS:HE2	1:A:2378:ILE:HG22	1.88	0.56
1:A:2025:ILE:HG23	1:A:2054:GLN:HE21	1.72	0.55
1:A:2159:ASN:HD22	1:A:2199:VAL:HG13	1.71	0.54
1:A:1847:ASP:O	1:A:1849:LYS:HG3	2.09	0.53
1:A:2003:THR:HG23	1:A:2324:VAL:HG23	1.89	0.53
1:A:1959:THR:HG22	1:A:1961:LEU:H	1.74	0.53
1:A:2025:ILE:HG23	1:A:2054:GLN:NE2	2.24	0.53
1:A:2250:THR:HA	1:A:2253:LEU:HD12	1.91	0.52
1:A:2076:GLN:NE2	1:A:2076:GLN:HA	2.24	0.52
1:A:2326:SER:HB3	1:A:2329:PHE:CB	2.40	0.51
1:A:2354:GLY:O	1:A:2355:ASN:HB2	2.11	0.51
1:A:1895:HIS:O	1:A:1898:VAL:HG22	2.11	0.51
1:A:2304:ALA:HB3	1:A:2337:ALA:O	2.10	0.50
1:A:2041:PRO:HB2	1:A:2043:PHE:CE2	2.46	0.50
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	1.94	0.50
1:A:1849:LYS:O	1:A:1850:LEU:HD23	2.11	0.50
1:A:2078:GLU:O	1:A:2082:ILE:HG13	2.13	0.49
1:A:2205:ALA:HB2	1:A:2226:LEU:HD12	1.94	0.49
1:A:1975:SER:O	1:A:1979:MET:HG2	2.13	0.49
1:A:2079:ILE:O	1:A:2083:ILE:HG13	2.13	0.48
1:A:2329:PHE:HA	1:A:2333:PHE:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1961:LEU:HD22	1:A:2084:LEU:HB3	1.94	0.48
1:A:1878:CYS:SG	1:A:1891:LEU:HD11	2.54	0.48
1:A:2326:SER:HB3	1:A:2329:PHE:HB3	1.96	0.48
1:A:1835:MET:HG2	1:A:1959:THR:HG23	1.95	0.47
1:A:2064:GLY:C	1:A:2068:ASN:HA	2.35	0.47
1:A:2254:GLU:O	1:A:2256:LEU:HD13	2.14	0.47
1:A:2213:LYS:HG2	1:A:2214:ASP:N	2.31	0.46
1:A:1925:PRO:HD2	1:A:1928:GLU:OE1	2.16	0.46
1:A:2214:ASP:O	1:A:2215:HIS:CB	2.63	0.46
1:A:2215:HIS:HA	1:A:2216:PRO:HD2	1.58	0.46
1:A:1859:ARG:NH1	1:A:1969:MET:HG2	2.30	0.45
1:A:1974:LEU:O	1:A:1977:VAL:HG22	2.18	0.44
1:A:2348:ASN:HD22	1:A:2348:ASN:C	2.21	0.44
1:A:2021:SER:O	1:A:2025:ILE:HG13	2.18	0.44
1:A:2168:ASN:HB2	1:A:2298:GLY:O	2.17	0.44
1:A:1867:GLU:HG3	1:A:1869:ASN:HB2	1.99	0.44
1:A:2225:VAL:HG11	1:A:2242:PRO:HG3	2.00	0.44
1:A:2247:LEU:HB2	1:A:2250:THR:HG21	1.99	0.43
1:A:2032:ILE:HG22	1:A:2032:ILE:O	2.17	0.43
1:A:2166:LEU:HD11	1:A:2191:LYS:HA	2.01	0.43
1:A:2228:PRO:HG2	1:A:2372:TYR:CD1	2.54	0.43
1:A:2177:VAL:H	1:A:2180:GLN:NE2	2.15	0.42
1:A:2226:LEU:O	1:A:2352:PRO:HD3	2.19	0.42
1:A:1893:ILE:HG21	1:A:1981:ALA:CB	2.50	0.42
1:A:2076:GLN:HE21	1:A:2079:ILE:HD12	1.84	0.42
1:A:2178:GLU:O	1:A:2217:LYS:HE2	2.19	0.42
1:A:2209:GLY:HA3	1:A:2220:GLU:O	2.20	0.42
1:A:1842:GLU:O	1:A:1845:ASN:ND2	2.53	0.42
1:A:2228:PRO:HD3	1:A:2352:PRO:HG3	2.02	0.41
1:A:2169:ILE:HG12	1:A:2300:VAL:HG22	2.02	0.41
1:A:2050:THR:O	1:A:2054:GLN:HG3	2.21	0.41
1:A:2176:PHE:HA	1:A:2180:GLN:HE22	1.86	0.41
1:A:2323:ASN:HB3	1:A:2324:VAL:H	1.57	0.40
1:A:1913:THR:O	1:A:1917:VAL:HG23	2.21	0.40
1:A:2302:LEU:N	1:A:2302:LEU:HD12	2.36	0.40
1:A:2318:ASN:HB3	1:A:2321:ILE:HG12	2.03	0.40
1:A:1837:SER:HA	1:A:1840:TYR:HB2	2.04	0.40
1:A:2162:LEU:HD21	1:A:2199:VAL:HG12	2.03	0.40

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	493/565 (87%)	447 (91%)	37 (8%)	9 (2%)	8 36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2068	ASN
1	A	2214	ASP
1	A	2284	LYS
1	A	2323	ASN
1	A	1900	ALA
1	A	1866	PHE
1	A	2029	ASP
1	A	2215	HIS
1	A	2322	MET

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	445/501 (89%)	419 (94%)	26 (6%)	20 50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1836	ASN
1	A	1839	ASN

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Mol	Chain	Res	Type
1	A	1867	GLU
1	A	1905	LEU
1	A	1906	SER
1	A	1931	LYS
1	A	1969	MET
1	A	1972	ASP
1	A	1982	THR
1	A	1986	MET
1	A	2001	SER
1	A	2002	TYR
1	A	2009	THR
1	A	2034	ILE
1	A	2036	SER
1	A	2057	ASP
1	A	2155	SER
1	A	2256	LEU
1	A	2296	THR
1	A	2310	GLU
1	A	2320	ASP
1	A	2325	LEU
1	A	2333	PHE
1	A	2348	ASN
1	A	2378	ILE
1	A	2381	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1839	ASN
1	A	1907	GLN
1	A	1990	ASN
1	A	2054	GLN
1	A	2070	ASN
1	A	2076	GLN
1	A	2159	ASN
1	A	2180	GLN
1	A	2237	GLN
1	A	2306	ASN
1	A	2348	ASN
1	A	2355	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 carbohydrates 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

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	497/565 (87%)	0.01	23 (4%) 32 30	13, 39, 85, 153	5 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1866	PHE	5.4
1	A	1868	GLY	4.1
1	A	1867	GLU	3.9
1	A	2150	ASN	3.7
1	A	1862	VAL	3.6
1	A	1869	ASN	3.1
1	A	1863	HIS	3.0
1	A	2068	ASN	2.9
1	A	2326	SER	2.7
1	A	1865	THR	2.7
1	A	1872	THR	2.6
1	A	2214	ASP	2.6
1	A	2149	LYS	2.6
1	A	1833	GLY	2.5
1	A	1864	LYS	2.4
1	A	2148	SER	2.4
1	A	1871	ALA	2.3
1	A	2151	GLU	2.3
1	A	2069	VAL	2.3
1	A	2324	VAL	2.2
1	A	2076	GLN	2.1
1	A	1861	THR	2.0
1	A	1960	GLU	2.0

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 carbohydrates 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.