



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:44 am BST

PDB ID : 3SBT
Title : Crystal structure of a Aar2-Prp8 complex
Authors : Weber, G.; Santos, K.F.; Holton, N.; Wahl, M.C.
Deposited on : 2011-06-06
Resolution : 1.80 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

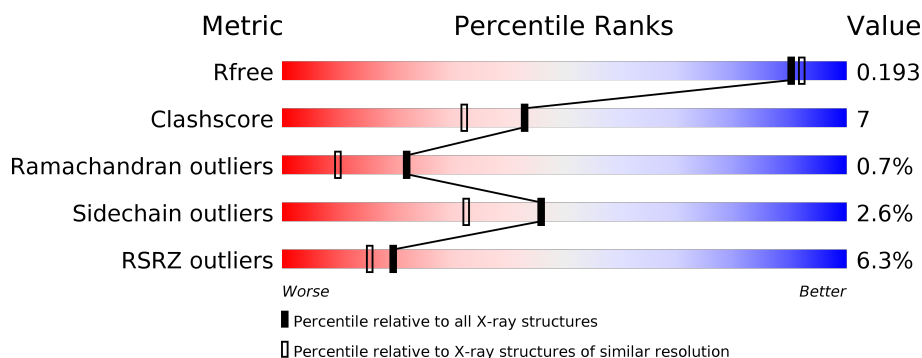
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	260	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
2	B	363	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>8%</div> <div>• •</div> <div>17%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5329 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
			Total	C	N	O	S			
1	A	253	2144	1373	361	400	10	1	13	0

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

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	300	2563	1642	418	484	19	0	8	0

There are 8 discrepancies between the modelled and reference sequences:

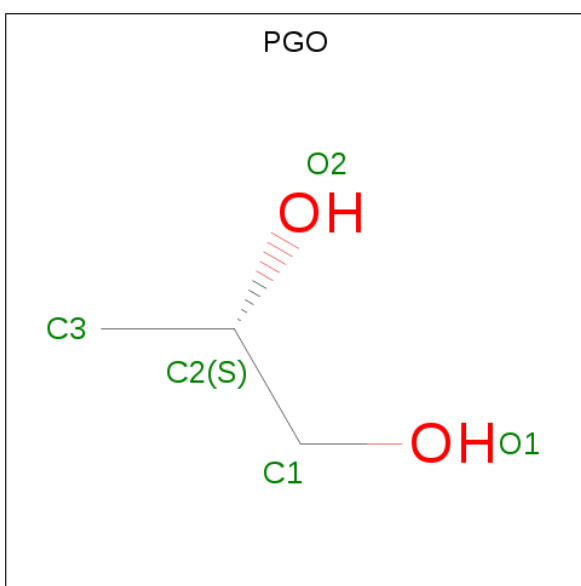
Chain	Residue	Modelled	Actual	Comment	Reference
B	356	LEU	-	EXPRESSION TAG	UNP P32357
B	357	GLU	-	EXPRESSION TAG	UNP P32357
B	358	HIS	-	EXPRESSION TAG	UNP P32357
B	359	HIS	-	EXPRESSION TAG	UNP P32357
B	360	HIS	-	EXPRESSION TAG	UNP P32357
B	361	HIS	-	EXPRESSION TAG	UNP P32357
B	362	HIS	-	EXPRESSION TAG	UNP P32357
B	363	HIS	-	EXPRESSION TAG	UNP P32357

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total 315	O 315	0	12
5	B	282	Total 292	O 292	0	10

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.33Å 82.02Å 94.06Å 90.00° 108.59° 90.00°	Depositor
Resolution (Å)	26.73 – 1.80 26.73 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (26.73-1.80) 99.6 (26.73-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.162 , 0.197 0.159 , 0.193	Depositor DCC
R_{free} test set	3000 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5329	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PGO, SO4

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	0.49	0/2185	0.61	0/2963
2	B	0.46	0/2629	0.59	0/3549
All	All	0.47	0/4814	0.60	0/6512

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	2144	0	2182	42	0
2	B	2563	0	2444	22	0
3	A	10	0	0	0	0
4	A	5	0	8	0	0
5	A	315	0	0	7	0
5	B	292	0	0	3	0
All	All	5329	0	4634	64	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 7.

All (64) 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:1962:ARG:HH11	1:A:1962:ARG:HG3	1.20	1.00
1:A:2060[B]:LEU:HD11	1:A:2079:ILE:HG23	1.43	1.00
1:A:2075:THR:HG22	1:A:2078:GLU:HG3	1.45	0.98
2:B:280:SER:HB2	2:B:313:TYR:CE1	2.15	0.82
2:B:148:GLN:O	2:B:153[A]:LEU:HA	1.87	0.74
1:A:2075:THR:HG23	1:A:2077:THR:H	1.52	0.73
1:A:1835:MET:SD	1:A:1843:LEU:HD21	2.28	0.73
2:B:108:ILE:HG13	2:B:108:ILE:O	1.90	0.70
1:A:1961:LEU:HD22	1:A:2086:GLN:HE21	1.56	0.69
1:A:1935:VAL:HG21	1:A:1941[A]:LEU:HD22	1.77	0.67
1:A:1962:ARG:CG	1:A:1962:ARG:HH11	2.00	0.67
1:A:2060[B]:LEU:CD1	1:A:2079:ILE:HG23	2.23	0.67
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.17	0.64
1:A:1962:ARG:NH1	1:A:1962:ARG:HG3	2.00	0.62
1:A:2075:THR:HG23	1:A:2077:THR:N	2.15	0.61
2:B:203:TYR:HD1	5:B:544:HOH:O	1.81	0.60
1:A:2075:THR:HG22	1:A:2078:GLU:H	1.67	0.59
1:A:2060[B]:LEU:HG	1:A:2083:ILE:HD11	1.82	0.59
1:A:2064:GLY:HA2	1:A:2069[B]:VAL:HG13	1.85	0.59
2:B:258:LYS:HE3	2:B:258:LYS:HA	1.85	0.59
1:A:2062:GLU:HG2	5:A:134:HOH:O	2.03	0.58
1:A:2060[A]:LEU:HD11	1:A:2074:LEU:HD23	1.85	0.57
1:A:2028:SER:HA	5:A:536:HOH:O	2.06	0.56
1:A:2064:GLY:HA2	1:A:2069[A]:VAL:HG22	1.87	0.56
2:B:50:ASP:HB3	5:B:497:HOH:O	2.05	0.56
2:B:92:ILE:HG22	2:B:93:VAL:N	2.21	0.55
2:B:107:LYS:O	2:B:108:ILE:HG23	2.07	0.54
2:B:32:GLY:C	2:B:102:MET:HE2	2.29	0.53
1:A:1938:LYS:HA	1:A:1941[A]:LEU:HD23	1.91	0.52
5:A:269:HOH:O	2:B:273:LYS:HE3	2.09	0.52
2:B:151:GLU:HG2	2:B:152:LEU:N	2.25	0.51
2:B:3:THR:HG23	2:B:102:MET:CE	2.41	0.51
1:A:2024:MET:O	1:A:2028:SER:HB3	2.10	0.51
1:A:1941[B]:LEU:O	1:A:1945:GLU:HG3	2.11	0.50
1:A:2075:THR:CG2	1:A:2078:GLU:HG3	2.30	0.49
1:A:1976[B]:ASP:OD1	1:A:1980:LYS:HE3	2.14	0.47
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.96	0.47
1:A:1961:LEU:HD22	1:A:2086:GLN:NE2	2.26	0.47
1:A:2046:GLU:HG2	1:A:2047:GLN:N	2.28	0.47
5:A:562:HOH:O	2:B:266:GLU:HG2	2.15	0.47
1:A:2084:LEU:O	1:A:2086:GLN:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1998:ARG:HD2	5:A:515:HOH:O	2.15	0.46
2:B:55:ARG:HB3	2:B:142[B]:SER:OG	2.15	0.46
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.15	0.46
2:B:148:GLN:HG3	2:B:153[A]:LEU:HG	1.99	0.46
2:B:64[A]:MET:SD	2:B:123:MET:HG2	2.56	0.45
1:A:2058:LEU:O	1:A:2058:LEU:HD23	2.16	0.45
1:A:2075:THR:CG2	1:A:2078:GLU:H	2.28	0.45
2:B:141:ASP:OD2	2:B:144:MET:HG3	2.17	0.45
1:A:1938:LYS:O	1:A:1941[A]:LEU:HD23	2.18	0.44
1:A:1962:ARG:CG	1:A:1962:ARG:NH1	2.67	0.43
5:A:345[B]:HOH:O	2:B:278:GLN:HG2	2.17	0.43
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.18	0.43
1:A:2017:THR:HG22	1:A:2062:GLU:HG3	2.00	0.43
2:B:16:GLY:HA3	2:B:45:HIS:CE1	2.53	0.42
1:A:1859:ARG:HD2	5:A:543:HOH:O	2.20	0.41
1:A:1967:ALA:HB2	1:A:2016:LYS:HB2	2.01	0.41
1:A:2058:LEU:C	1:A:2058:LEU:CD2	2.87	0.41
1:A:2023:LYS:O	1:A:2027:LEU:HD22	2.21	0.41
2:B:33:ILE:N	2:B:102:MET:HE2	2.36	0.41
2:B:122:GLN:HG3	5:B:609:HOH:O	2.21	0.41
2:B:263:LYS:HD2	2:B:263:LYS:HA	1.87	0.41
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	2.03	0.40
1:A:2084:LEU:O	1:A:2086:GLN:N	2.53	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	264/260 (102%)	259 (98%)	4 (2%)	1 (0%)	34 21
2	B	303/363 (84%)	291 (96%)	9 (3%)	3 (1%)	15 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	567/623 (91%)	550 (97%)	13 (2%)	4 (1%)	22 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2085	GLY
2	B	107	LYS
2	B	151	GLU
2	B	108	ILE

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	243/235 (103%)	236 (97%)	7 (3%)	42 29
2	B	287/334 (86%)	280 (98%)	7 (2%)	49 36
All	All	530/569 (93%)	516 (97%)	14 (3%)	46 32

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1962	ARG
1	A	1985[A]	GLN
1	A	1985[B]	GLN
1	A	1988	LEU
1	A	2046	GLU
1	A	2075	THR
2	B	107	LYS
2	B	108	ILE
2	B	152	LEU
2	B	241	LEU
2	B	258	LYS
2	B	316	LEU
2	B	317	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2054	GLN
1	A	2086	GLN
2	B	23	ASN
2	B	150	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	2	-	4,4,4	0.13	0	6,6,6	0.19	0
3	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.09	0
4	PGO	A	2093	-	3,4,4	0.86	0	1,4,4	0.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGO	A	2093	-	-	0/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	253/260 (97%)	0.02	16 (6%)	20 15	18, 29, 73, 106	1 (0%)
2	B	300/363 (82%)	0.15	19 (6%)	20 15	18, 34, 68, 108	0
All	All	553/623 (88%)	0.09	35 (6%)	20 15	18, 32, 69, 108	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	153[A]	LEU	7.5
2	B	152	LEU	7.2
2	B	109	ASP	6.5
2	B	108	ILE	5.5
2	B	1	MET	5.3
1	A	2071	ILE	5.2
2	B	172	PRO	3.9
2	B	224	LEU	3.8
1	A	2077	THR	3.6
1	A	2079	ILE	3.5
1	A	2076	GLN	3.3
2	B	279	TYR	3.3
2	B	150	ASN	3.1
1	A	2082	ILE	2.8
1	A	2086	GLN	2.7
2	B	316	LEU	2.7
2	B	121	VAL	2.7
1	A	1880	PHE	2.7
2	B	110	GLU	2.6
1	A	1836	ASN	2.5
1	A	1882	LEU	2.5
2	B	247	ILE	2.4
2	B	315	GLU	2.3
2	B	229	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2083	ILE	2.3
2	B	281	ASP	2.3
1	A	1834	ALA	2.2
2	B	278	GLN	2.2
1	A	1838	SER	2.2
2	B	84	ARG	2.1
1	A	1965	PHE	2.1
1	A	1837	SER	2.1
2	B	228	PHE	2.1
1	A	2072	SER	2.1
1	A	1962	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	2	5/5	0.95	0.17	72,73,75,76	0
4	PGO	A	2093	5/5	0.95	0.12	31,34,36,38	0
3	SO4	A	1	5/5	0.98	0.14	38,54,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.