Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 08:51 am BST

PDB ID	:	2AFC
Title	:	X-Ray Crystal Structure of Protein Q8A8B0 from Bacteroides thetaiotaomicron. Northeast Structural Genomics Consortium Target BtR9.
Authors	:	Kuzin, A.P.; Abashidze, M.; Vorobiev, S.M.; Acton, T.; Xiao, R.; Conover, K.; Ma, L.-C.; Cunninggham, K.E.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-07-25
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

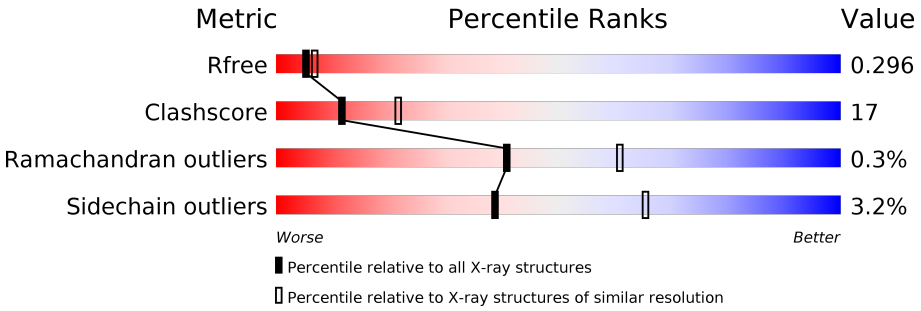
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	168	64% 25% • 9%
1	B	168	61% 29% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2544 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 conserved hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	Se	0	0	0
			1206	782	202	215	3	4			
1	B	153	Total	C	N	O	S	Se	0	0	0
			1206	782	202	215	3	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
A	45	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
A	79	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
A	120	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
A	135	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
A	156	MSE	-	CLONING ARTIFACT	UNP Q8A8B0
A	157	ALA	-	CLONING ARTIFACT	UNP Q8A8B0
A	158	GLY	-	CLONING ARTIFACT	UNP Q8A8B0
A	159	ASP	-	CLONING ARTIFACT	UNP Q8A8B0
A	160	PRO	-	CLONING ARTIFACT	UNP Q8A8B0
A	161	LEU	-	CLONING ARTIFACT	UNP Q8A8B0
A	162	GLU	-	CLONING ARTIFACT	UNP Q8A8B0
A	163	HIS	-	EXPRESSION TAG	UNP Q8A8B0
A	164	HIS	-	EXPRESSION TAG	UNP Q8A8B0
A	165	HIS	-	EXPRESSION TAG	UNP Q8A8B0
A	166	HIS	-	EXPRESSION TAG	UNP Q8A8B0
A	167	HIS	-	EXPRESSION TAG	UNP Q8A8B0
A	168	HIS	-	EXPRESSION TAG	UNP Q8A8B0
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
B	45	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
B	79	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
B	120	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
B	135	MSE	MET	MODIFIED RESIDUE	UNP Q8A8B0
B	156	MSE	-	CLONING ARTIFACT	UNP Q8A8B0
B	157	ALA	-	CLONING ARTIFACT	UNP Q8A8B0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	158	GLY	-	CLONING ARTIFACT	UNP Q8A8B0
B	159	ASP	-	CLONING ARTIFACT	UNP Q8A8B0
B	160	PRO	-	CLONING ARTIFACT	UNP Q8A8B0
B	161	LEU	-	CLONING ARTIFACT	UNP Q8A8B0
B	162	GLU	-	CLONING ARTIFACT	UNP Q8A8B0
B	163	HIS	-	EXPRESSION TAG	UNP Q8A8B0
B	164	HIS	-	EXPRESSION TAG	UNP Q8A8B0
B	165	HIS	-	EXPRESSION TAG	UNP Q8A8B0
B	166	HIS	-	EXPRESSION TAG	UNP Q8A8B0
B	167	HIS	-	EXPRESSION TAG	UNP Q8A8B0
B	168	HIS	-	EXPRESSION TAG	UNP Q8A8B0

- Molecule 2 is water.

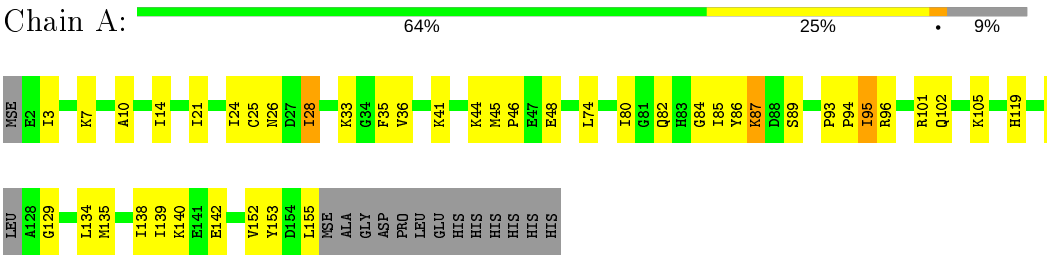
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total O 69 69	0	0
2	B	63	Total O 63 63	0	0

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. 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. 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.

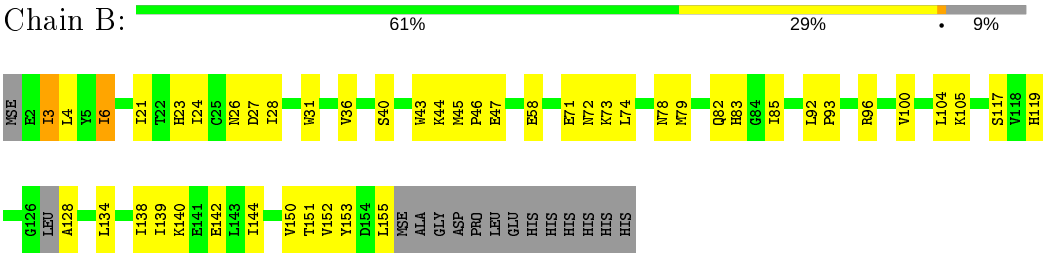
- Molecule 1: conserved hypothetical protein

Chain A:



- Molecule 1: conserved hypothetical protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.44Å 36.44Å 84.03Å 90.00° 129.03° 90.00°	Depositor
Resolution (Å)	27.61 – 2.50 27.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (27.61-2.50) 92.3 (27.61-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	6.23 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.288 0.223 , 0.296	Depositor DCC
R_{free} test set	2397 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2544	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.38	0/1228	0.60	0/1649
1	B	0.36	0/1228	0.59	0/1649
All	All	0.37	0/2456	0.60	0/3298

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	1206	0	1228	38	0
1	B	1206	0	1228	51	0
2	A	69	0	0	2	0
2	B	63	0	0	6	0
All	All	2544	0	2456	85	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 17.

All (85) 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:3:ILE:HD11	1:A:152:VAL:HG23	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HD13	1:A:84:GLY:HA2	1.62	0.81
1:A:21:ILE:HD11	1:A:74:LEU:HD11	1.60	0.81
1:B:120:MSE:CE	1:B:123:ILE:HG12	2.13	0.77
1:B:3:ILE:HD13	1:B:150:VAL:HG12	1.67	0.77
1:A:95:ILE:HD13	1:A:96:ARG:N	2.00	0.77
1:A:3:ILE:HD11	1:A:152:VAL:CG2	2.14	0.76
1:B:24:ILE:HD13	1:B:79:MSE:HE3	1.67	0.74
1:B:6:ILE:HD11	1:B:153:TYR:CD2	2.25	0.71
1:B:3:ILE:HD11	1:B:152:VAL:HG23	1.72	0.71
1:B:24:ILE:CD1	1:B:79:MSE:HE3	2.22	0.69
1:B:120:MSE:HE1	1:B:123:ILE:HG12	1.74	0.69
1:A:14:ILE:HD11	2:A:200:HOH:O	1.93	0.68
1:B:120:MSE:HE3	1:B:123:ILE:HG23	1.77	0.66
1:A:25:CYS:HB2	1:A:80:ILE:HD13	1.77	0.66
1:A:93:PRO:HB3	1:A:129:GLY:HA3	1.80	0.64
1:A:21:ILE:CD1	1:A:74:LEU:HD11	2.28	0.62
1:B:120:MSE:HE3	1:B:123:ILE:HG12	1.81	0.62
1:B:140:LYS:HA	1:B:144:ILE:HB	1.82	0.61
1:B:3:ILE:CD1	1:B:152:VAL:HG23	2.30	0.60
1:B:40:SER:HA	1:B:43:TRP:O	2.01	0.59
1:B:96:ARG:O	1:B:100:VAL:HG23	2.04	0.58
1:A:135:MSE:O	1:A:139:ILE:HG12	2.04	0.56
1:B:104:LEU:HD13	1:B:139:ILE:HD13	1.87	0.56
1:B:45:MSE:HB3	1:B:46:PRO:HD3	1.86	0.56
1:B:31:TRP:CE2	1:B:36:VAL:HB	2.41	0.55
1:B:85:ILE:O	1:B:85:ILE:HG22	2.06	0.55
1:A:21:ILE:N	1:A:21:ILE:HD12	2.22	0.55
1:A:102:GLN:HG2	1:B:92:LEU:HD11	1.90	0.54
1:B:71:GLU:HG3	1:B:74:LEU:HD23	1.90	0.53
1:A:138:ILE:HD11	1:B:134:LEU:HD21	1.90	0.53
1:B:104:LEU:CD1	1:B:139:ILE:HD13	2.39	0.52
1:A:86:TYR:C	1:A:87:LYS:HD2	2.30	0.52
1:B:6:ILE:HD11	1:B:153:TYR:CG	2.45	0.52
1:A:140:LYS:HE2	2:B:228:HOH:O	2.11	0.51
1:A:105:LYS:HE3	1:A:142:GLU:OE1	2.10	0.51
1:A:7:LYS:HD3	1:A:155:LEU:O	2.11	0.51
1:A:24:ILE:HD12	1:A:124:GLY:N	2.25	0.50
1:B:3:ILE:HD11	1:B:152:VAL:H	1.75	0.50
1:B:26:ASN:HA	1:B:82:GLN:HB3	1.92	0.50
1:B:31:TRP:CE2	1:B:47:GLU:HB2	2.47	0.49
1:B:36:VAL:HG13	2:B:175:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:C	1:A:85:ILE:HD12	2.34	0.49
1:B:28:ILE:HG12	1:B:28:ILE:O	2.13	0.48
1:B:6:ILE:HD13	1:B:6:ILE:H	1.78	0.48
1:B:119:HIS:HD2	1:B:153:TYR:OH	1.97	0.48
1:B:117:SER:HB3	1:B:119:HIS:HE1	1.78	0.47
1:B:3:ILE:HD12	1:B:150:VAL:O	2.14	0.47
1:A:86:TYR:O	1:A:94:PRO:HD3	2.15	0.47
1:A:26:ASN:HA	1:A:82:GLN:HB3	1.97	0.47
1:B:3:ILE:HD12	1:B:4:LEU:N	2.31	0.46
1:A:87:LYS:HD2	1:A:87:LYS:N	2.30	0.46
1:B:123:ILE:O	1:B:123:ILE:HG13	2.16	0.46
1:A:95:ILE:HD13	1:A:95:ILE:C	2.36	0.46
1:B:6:ILE:HD12	1:B:151:THR:CG2	2.46	0.45
1:B:23:HIS:HE1	1:B:78:ASN:OD1	1.98	0.45
1:A:119:HIS:HD2	1:A:153:TYR:OH	1.99	0.45
1:B:44:LYS:HE2	2:B:193:HOH:O	2.17	0.45
1:B:93:PRO:HB2	1:B:128:ALA:O	2.18	0.44
1:A:3:ILE:HD11	1:A:152:VAL:HG21	1.97	0.44
1:B:21:ILE:HA	1:B:119:HIS:O	2.18	0.43
1:B:3:ILE:HD11	1:B:152:VAL:N	2.33	0.43
1:A:41:LYS:HD3	2:A:207:HOH:O	2.17	0.43
1:A:33:LYS:O	1:A:36:VAL:HG22	2.19	0.43
1:B:6:ILE:HD11	1:B:153:TYR:CE2	2.53	0.43
1:B:6:ILE:HD12	1:B:151:THR:HG22	2.00	0.43
1:A:21:ILE:HA	1:A:119:HIS:O	2.19	0.42
1:B:23:HIS:HD2	2:B:206:HOH:O	2.02	0.42
1:A:105:LYS:NZ	1:B:92:LEU:HD23	2.34	0.42
1:B:122:ARG:NE	2:B:189:HOH:O	2.51	0.42
1:A:10:ALA:HB3	1:A:35:PHE:CE1	2.55	0.42
1:A:24:ILE:CD1	1:A:123:ILE:HB	2.49	0.42
1:B:3:ILE:HD13	1:B:150:VAL:CG1	2.44	0.41
1:B:71:GLU:HB2	1:B:74:LEU:HB3	2.03	0.41
1:B:27:ASP:OD2	1:B:83:HIS:HD2	2.03	0.41
1:A:123:ILE:O	1:A:123:ILE:HG13	2.20	0.41
1:A:101:ARG:CG	1:A:138:ILE:HD12	2.51	0.41
1:B:93:PRO:HG2	2:B:176:HOH:O	2.20	0.41
1:A:134:LEU:HD21	1:B:138:ILE:HG12	2.03	0.41
1:B:72:ASN:ND2	1:B:73:LYS:HG3	2.35	0.41
1:A:124:GLY:HA3	1:A:135:MSE:HE3	2.04	0.40
1:B:105:LYS:HD2	1:B:142:GLU:OE1	2.22	0.40
1:A:95:ILE:HD13	1:A:96:ARG:C	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MSE:HB2	1:A:46:PRO:HD3	2.03	0.40
1:A:48:GLU:HA	1:A:48:GLU:OE2	2.22	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	149/168 (89%)	136 (91%)	12 (8%)	1 (1%)	22 39
1	B	149/168 (89%)	141 (95%)	8 (5%)	0	100 100
All	All	298/336 (89%)	277 (93%)	20 (7%)	1 (0%)	41 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	SER

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	126/133 (95%)	122 (97%)	4 (3%)	39 65
1	B	126/133 (95%)	122 (97%)	4 (3%)	39 65
All	All	252/266 (95%)	244 (97%)	8 (3%)	39 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	44	LYS
1	A	87	LYS
1	A	95	ILE
1	B	3	ILE
1	B	6	ILE
1	B	58	GLU
1	B	155	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	69	ASN
1	A	83	HIS
1	A	119	HIS
1	B	23	HIS
1	B	69	ASN
1	B	72	ASN
1	B	83	HIS
1	B	119	HIS

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 carbohydrates 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.