



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2023 – 05:22 PM EDT

PDB ID : 5DIH
Title : Structure of Haliangium ochraceum BMC-T HO-5812
Authors : Sutter, M.; Aussignargues, C.; Turmo, A.; Kerfeld, C.A.
Deposited on : 2015-09-01
Resolution : 2.44 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
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

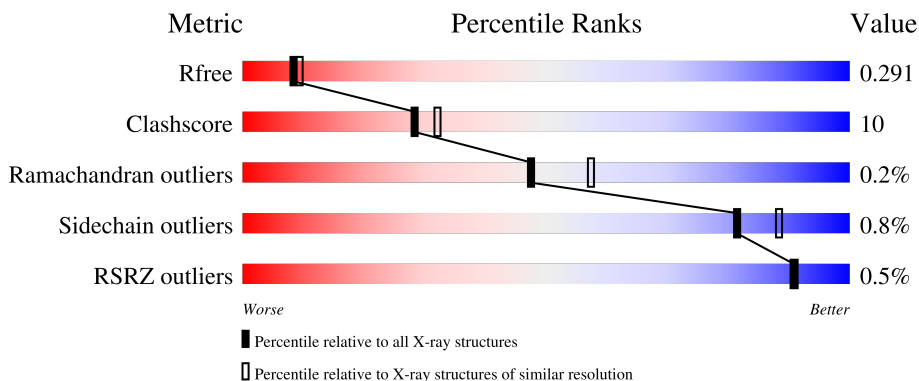
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	205	 2% 78% 20% .
1	B	205	 77% 21% .
1	C	205	 74% 19% 7%
1	D	205	 76% 13% 11%
1	E	205	 72% 20% . 6%

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Mol	Chain	Length	Quality of chain
1	F	205	 75% 18% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9018 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 Microcompartments protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	Total 1503	C 949	N 263	O 283	S 8	0	0	0
1	B	202	Total 1510	C 953	N 264	O 284	S 9	0	0	0
1	C	191	Total 1433	C 906	N 251	O 268	S 8	0	0	0
1	D	182	Total 1363	C 864	N 239	O 252	S 8	0	0	0
1	E	192	Total 1444	C 915	N 252	O 269	S 8	0	0	0
1	F	192	Total 1434	C 906	N 251	O 269	S 8	0	0	0

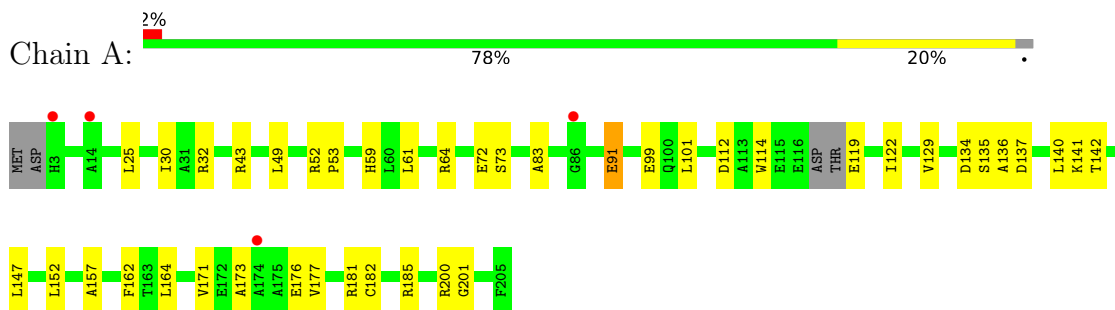
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total 55	O 55	0	0
2	B	58	Total 58	O 58	0	0
2	C	66	Total 66	O 66	0	0
2	D	57	Total 57	O 57	0	0
2	E	51	Total 51	O 51	0	0
2	F	44	Total 44	O 44	0	0

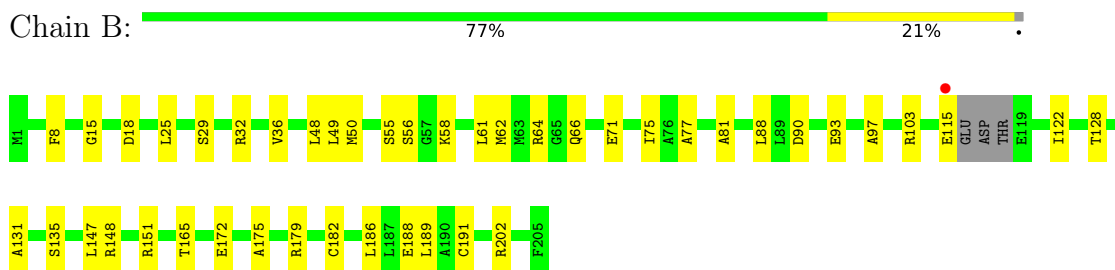
3 Residue-property plots

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.

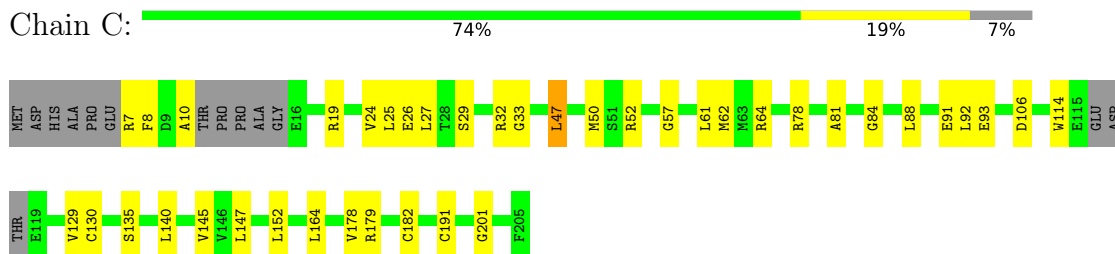
- Molecule 1: Microcompartments protein



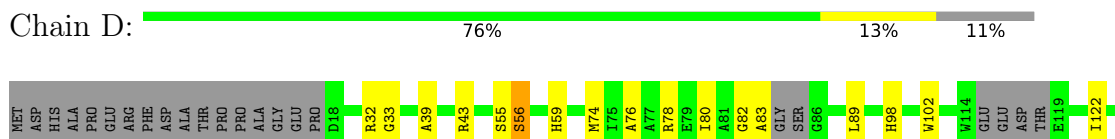
- Molecule 1: Microcompartments protein



- Molecule 1: Microcompartments protein



- Molecule 1: Microcompartments protein





- Molecule 1: Microcompartments protein

Chain E: 72% 20% 6%



- Molecule 1: Microcompartments protein

Chain F: 75% 18% 6%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.63Å 66.38Å 122.25Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	31.51 – 2.44 30.81 – 2.44	Depositor EDS
% Data completeness (in resolution range)	91.7 (31.51-2.44) 87.8 (30.81-2.44)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.233 , 0.277 0.247 , 0.291	Depositor DCC
R_{free} test set	1868 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtrriage
Anisotropy	1.265	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9018	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6759e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.23	0/1526	0.38	0/2072
1	B	0.25	0/1533	0.39	0/2081
1	C	0.25	0/1451	0.38	0/1965
1	D	0.23	0/1379	0.38	0/1868
1	E	0.26	0/1463	0.42	0/1983
1	F	0.24	0/1452	0.41	0/1968
All	All	0.24	0/8804	0.39	0/11937

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	1503	0	1528	31	0
1	B	1510	0	1538	37	0
1	C	1433	0	1467	28	0
1	D	1363	0	1409	20	0
1	E	1444	0	1479	35	0
1	F	1434	0	1473	28	0
2	A	55	0	0	8	0
2	B	58	0	0	18	0
2	C	66	0	0	10	0
2	D	57	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	51	0	0	11	0
2	F	44	0	0	11	0
All	All	9018	0	8894	173	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 173 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:B:15:GLY:CA	2:B:302:HOH:O	2.20	0.90
1:B:55:SER:O	1:B:56:SER:OG	1.91	0.88
1:E:55:SER:O	1:E:56:SER:OG	1.93	0.86
1:B:15:GLY:N	2:B:302:HOH:O	2.08	0.85
1:D:55:SER:O	1:D:56:SER:OG	1.94	0.84

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	197/205 (96%)	189 (96%)	8 (4%)	0	100	100
1	B	198/205 (97%)	187 (94%)	11 (6%)	0	100	100
1	C	185/205 (90%)	171 (92%)	13 (7%)	1 (0%)	29	34
1	D	176/205 (86%)	163 (93%)	12 (7%)	1 (1%)	25	29
1	E	184/205 (90%)	174 (95%)	10 (5%)	0	100	100
1	F	186/205 (91%)	172 (92%)	14 (8%)	0	100	100
All	All	1126/1230 (92%)	1056 (94%)	68 (6%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	56	SER
1	C	84	GLY

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	152/156 (97%)	150 (99%)	2 (1%)	69	80
1	B	153/156 (98%)	153 (100%)	0	100	100
1	C	145/156 (93%)	144 (99%)	1 (1%)	84	90
1	D	138/156 (88%)	138 (100%)	0	100	100
1	E	147/156 (94%)	145 (99%)	2 (1%)	67	78
1	F	146/156 (94%)	144 (99%)	2 (1%)	67	78
All	All	881/936 (94%)	874 (99%)	7 (1%)	81	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	27	LEU
1	E	122	ILE
1	F	172	GLU
1	F	112	ASP
1	C	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	GLN

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 monosaccharides 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 [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	201/205 (98%)	-0.24	4 (1%) 65 61	22, 35, 60, 74	0
1	B	202/205 (98%)	-0.30	1 (0%) 91 91	23, 38, 53, 68	0
1	C	191/205 (93%)	-0.26	0 100 100	26, 37, 51, 68	0
1	D	182/205 (88%)	-0.27	0 100 100	26, 36, 48, 56	0
1	E	192/205 (93%)	-0.24	0 100 100	28, 38, 59, 76	0
1	F	192/205 (93%)	-0.19	1 (0%) 91 91	31, 40, 58, 77	0
All	All	1160/1230 (94%)	-0.25	6 (0%) 91 91	22, 37, 56, 77	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	15	GLY	5.0
1	A	174	ALA	2.7
1	A	14	ALA	2.5
1	B	115	GLU	2.2
1	A	86	GLY	2.2

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.