Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:50 AM EDT

PDB ID	:	6MCJ
Title	:	Structure of Helical Carotenoid Protein 2 from Fremyella diplosiphon
Authors	:	Sutter, M.; Dominguez-Martin, M.A.
Deposited on	:	2018-08-31
Resolution	:	1.71 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 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 (i)

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

The reported resolution of this entry is 1.71 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4951 atoms, of which 2377 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 Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	H	N	O	S	0	0	0
			2274	726	1125	197	222	4			
1	B	145	Total	C	H	N	O	S	0	0	0
			2275	726	1126	197	222	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	GLY	-	expression tag	UNP A0A0D6L0Q7
A	150	SER	-	expression tag	UNP A0A0D6L0Q7
A	151	SER	-	expression tag	UNP A0A0D6L0Q7
A	152	ALA	-	expression tag	UNP A0A0D6L0Q7
A	153	HIS	-	expression tag	UNP A0A0D6L0Q7
A	154	HIS	-	expression tag	UNP A0A0D6L0Q7
A	155	HIS	-	expression tag	UNP A0A0D6L0Q7
A	156	HIS	-	expression tag	UNP A0A0D6L0Q7
A	157	HIS	-	expression tag	UNP A0A0D6L0Q7
A	158	HIS	-	expression tag	UNP A0A0D6L0Q7
A	159	HIS	-	expression tag	UNP A0A0D6L0Q7
A	160	HIS	-	expression tag	UNP A0A0D6L0Q7
A	161	HIS	-	expression tag	UNP A0A0D6L0Q7
A	162	HIS	-	expression tag	UNP A0A0D6L0Q7
B	149	GLY	-	expression tag	UNP A0A0D6L0Q7
B	150	SER	-	expression tag	UNP A0A0D6L0Q7
B	151	SER	-	expression tag	UNP A0A0D6L0Q7
B	152	ALA	-	expression tag	UNP A0A0D6L0Q7
B	153	HIS	-	expression tag	UNP A0A0D6L0Q7
B	154	HIS	-	expression tag	UNP A0A0D6L0Q7
B	155	HIS	-	expression tag	UNP A0A0D6L0Q7
B	156	HIS	-	expression tag	UNP A0A0D6L0Q7
B	157	HIS	-	expression tag	UNP A0A0D6L0Q7
B	158	HIS	-	expression tag	UNP A0A0D6L0Q7
B	159	HIS	-	expression tag	UNP A0A0D6L0Q7

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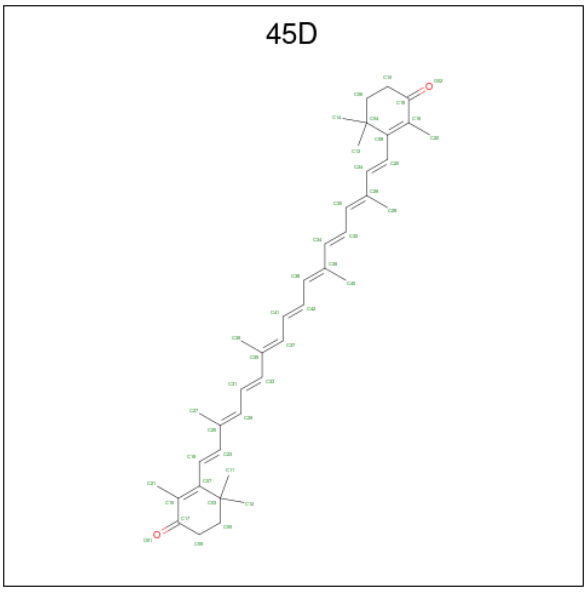
Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	-	expression tag	UNP A0A0D6L0Q7
B	161	HIS	-	expression tag	UNP A0A0D6L0Q7
B	162	HIS	-	expression tag	UNP A0A0D6L0Q7

- Molecule 2 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).

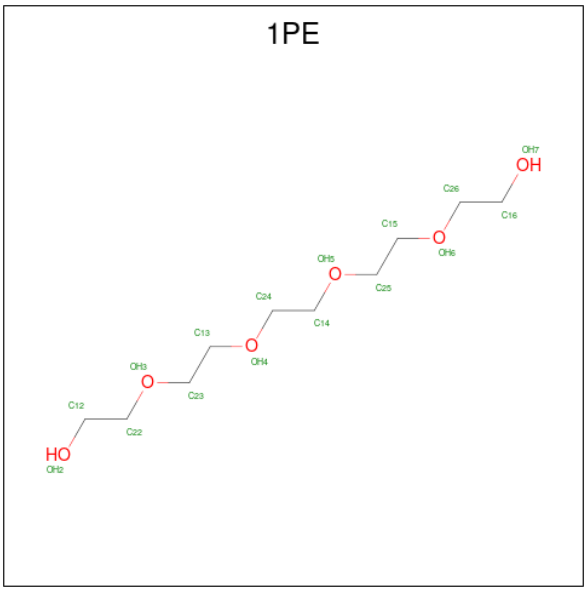


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 94 40 52 2	0	0
2	B	1	Total C H O 94 40 52 2	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total I 4 4	0	0
3	B	4	Total I 4 4	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	B	73	Total	O	0	0
			73	73		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	35.16Å 71.64Å 56.34Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	44.26 – 1.71	Depositor
% Data completeness (in resolution range)	94.0 (44.26-1.71)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 1.71Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.167 , 0.199	Depositor
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.187	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
Total number of atoms	4951	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.67% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
4	1PE	A	206	-	15,15,15	0.53	0	14,14,14	0.31	0
2	45D	B	201	-	43,43,43	0.83	1 (2%)	54,60,60	1.72	15 (27%)
2	45D	A	201	-	43,43,43	0.79	0	54,60,60	1.78	13 (24%)

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	1PE	A	206	-	-	8/13/13/13	-
2	45D	B	201	-	-	2/29/69/69	0/2/2/2
2	45D	A	201	-	-	3/29/69/69	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	45D	C04-C08	-2.78	1.49	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	45D	C05-C09-C17	-4.39	105.00	112.85
2	B	201	45D	C05-C09-C17	-4.01	105.67	112.85
2	B	201	45D	C06-C04-C08	-3.53	105.05	110.48
2	B	201	45D	C23-C25-C29	3.42	124.19	118.94
2	A	201	45D	C23-C25-C29	3.30	124.01	118.94
2	A	201	45D	C33-C35-C37	3.21	123.87	118.94
2	A	201	45D	C09-C17-C15	-3.15	115.75	118.65
2	A	201	45D	C06-C10-C18	-2.99	107.50	112.85
2	B	201	45D	C24-C26-C30	2.98	123.51	118.94
2	A	201	45D	C24-C26-C30	2.76	123.17	118.94
2	B	201	45D	C33-C35-C37	2.73	123.13	118.94
2	B	201	45D	C13-C04-C08	2.70	114.68	110.30
2	A	201	45D	C42-C41-C37	2.61	128.82	123.47
2	B	201	45D	C42-C38-C36	2.53	130.93	127.31
2	A	201	45D	C13-C04-C08	2.50	114.36	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	45D	C09-C17-C15	-2.50	116.35	118.65
2	B	201	45D	C41-C37-C35	2.44	130.79	127.31
2	A	201	45D	C20-C24-C26	2.39	129.84	126.23
2	B	201	45D	C34-C36-C38	2.36	122.56	118.94
2	A	201	45D	C42-C38-C36	2.35	130.67	127.31
2	B	201	45D	C42-C41-C37	2.26	128.09	123.47
2	A	201	45D	C32-C30-C26	2.24	130.50	127.31
2	B	201	45D	C27-C25-C29	-2.23	119.80	122.92
2	B	201	45D	C10-C06-C04	-2.23	109.60	113.18
2	A	201	45D	C34-C36-C38	2.22	122.36	118.94
2	B	201	45D	C06-C10-C18	-2.19	108.93	112.85
2	B	201	45D	C32-C30-C26	2.02	130.20	127.31
2	A	201	45D	C32-C34-C36	2.02	132.10	126.42

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	206	1PE	OH5-C14-C24-OH4
4	A	206	1PE	OH6-C15-C25-OH5
2	A	201	45D	C03-C07-C19-C23
2	B	201	45D	C03-C07-C19-C23
4	A	206	1PE	OH2-C12-C22-OH3
4	A	206	1PE	C25-C15-OH6-C26
4	A	206	1PE	C23-C13-OH4-C24
4	A	206	1PE	C13-C23-OH3-C22
4	A	206	1PE	C15-C25-OH5-C14
2	A	201	45D	C04-C08-C20-C24
2	B	201	45D	C15-C07-C19-C23
4	A	206	1PE	C12-C22-OH3-C23
2	A	201	45D	C15-C07-C19-C23

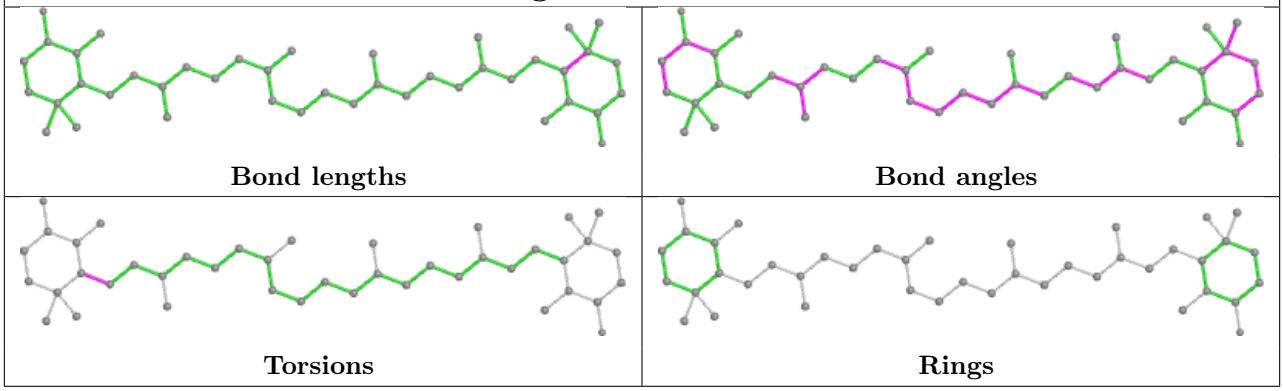
There are no ring outliers.

No monomer is involved in short contacts.

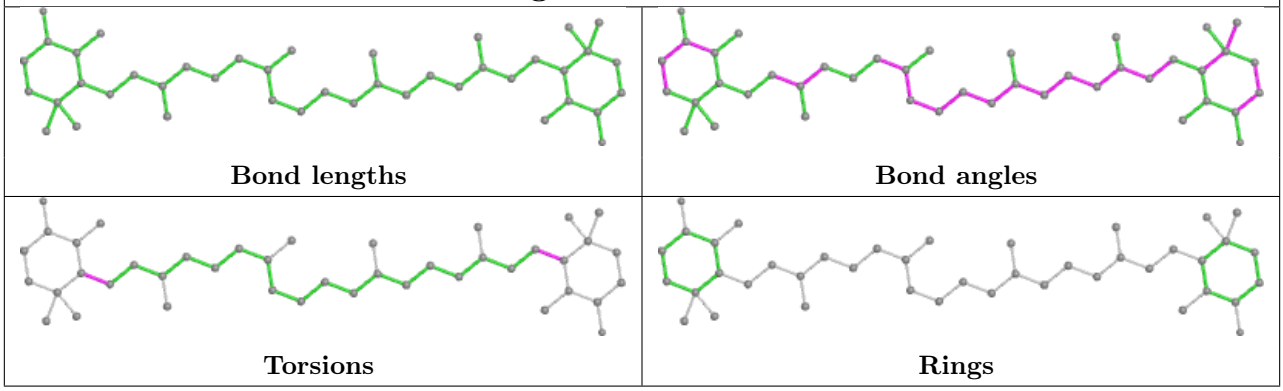
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 45D B 201



Ligand 45D A 201



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.