WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 30, 2023 – 08:03 am GMT

PDB ID	:	8PYH
Title	:	Crystal structure of the Orange Carotenoid Protein 2 (OCP2) from Crinalium epipsammum PCC 9333
Authors	:	Boyko, K.M.; Varfolomeeva, L.A.; Slonimskiy, Y.B.; Maksimov, E.G.; Popov, V.O.; Sluchanko, N.N.
Deposited on	:	2023-07-25
Resolution	:	2.20 Å(reported)

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

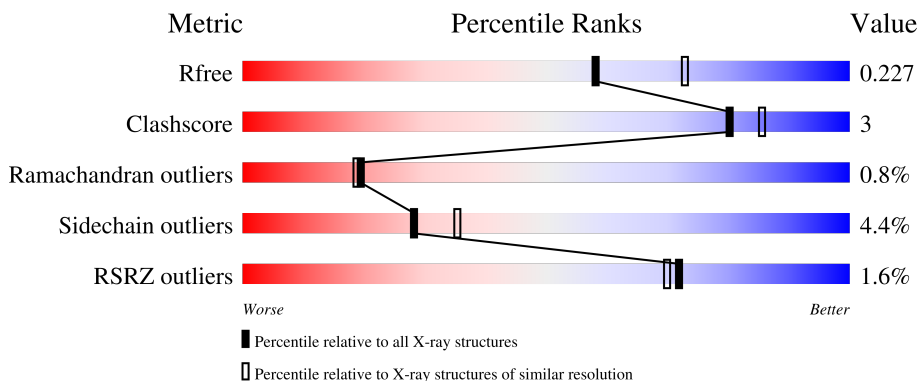|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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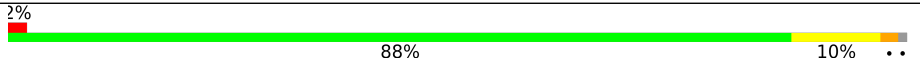*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		4.4%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	321	87% 9%
1	B	321	88% 10%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5285 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 Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	5	0
			2428	1549	393	470	16			
1	B	319	Total	C	N	O	S	0	8	0
			2468	1575	397	480	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP K9VSN3
A	0	HIS	-	expression tag	UNP K9VSN3
A	26	ALA	GLU	engineered mutation	UNP K9VSN3
B	-1	SER	-	expression tag	UNP K9VSN3
B	0	HIS	-	expression tag	UNP K9VSN3
B	26	ALA	GLU	engineered mutation	UNP K9VSN3

- Molecule 2 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).

ECH
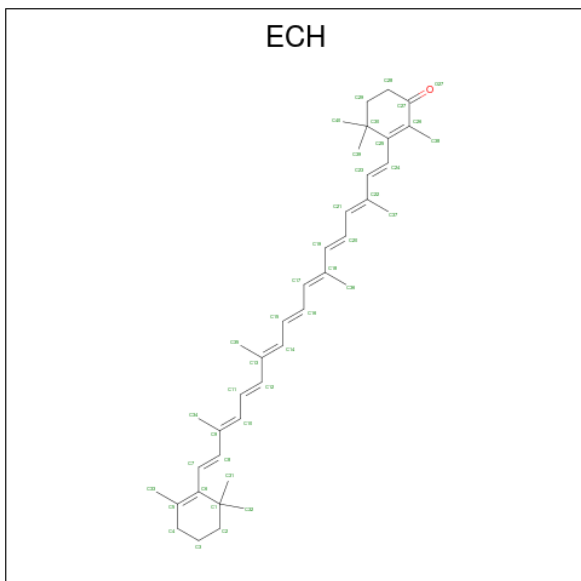
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total C O 41 40 1			0	0
2	B	1	Total C O 41 40 1			0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total O 169 169		0	0
4	B	134	Total O 134 134		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: Orange carotenoid-binding protein
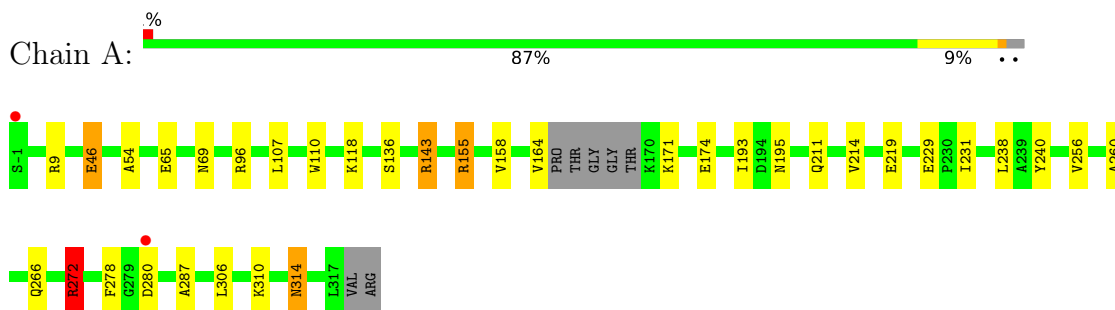
• Molecule 1: Orange carotenoid-binding protein
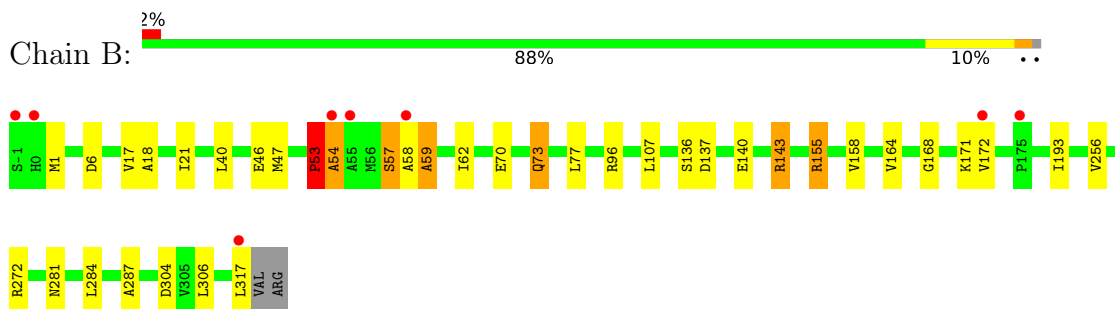
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.05Å 103.73Å 109.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.20 – 2.20 22.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.5 (22.20-2.20) 85.3 (22.20-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.177 , 0.227 0.181 , 0.227	Depositor DCC
R_{free} test set	1824 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 14.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.33, < L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5285	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.64	3/2492 (0.1%)	1.03	9/3389 (0.3%)
1	B	0.62	0/2547	1.00	2/3467 (0.1%)
All	All	0.63	3/5039 (0.1%)	1.01	11/6856 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	9
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CD-OE2	-6.15	1.18	1.25
1	A	46	GLU	CD-OE2	-5.48	1.19	1.25
1	A	229	GLU	CD-OE2	-5.34	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	B	53	PRO	N-CA-CB	-9.51	91.89	103.30
1	A	155	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	B	53	PRO	N-CD-CG	-7.83	91.45	103.20
1	A	272	ARG	CB-CA-C	7.78	125.96	110.40
1	A	278	PHE	CB-CA-C	-6.20	98.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	LYS	CB-CA-C	-5.74	98.92	110.40
1	A	272	ARG	N-CA-CB	-5.70	100.34	110.60
1	A	272	ARG	CG-CD-NE	5.41	123.16	111.80
1	A	46	GLU	CB-CA-C	-5.25	99.89	110.40
1	A	9	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	143	ARG	Sidechain
1	B	155	ARG	Sidechain
1	B	171	LYS	Peptide
1	B	172	VAL	Peptide
1	B	47	MET	Peptide
1	B	54	ALA	Peptide
1	B	58	ALA	Peptide
1	B	59	ALA	Peptide
1	B	96	ARG	Sidechain

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	2428	0	2380	11	0
1	B	2468	0	2413	13	0
2	A	41	0	54	3	0
2	B	41	0	54	3	0
3	A	4	0	3	0	0
4	A	169	0	0	0	0
4	B	134	0	0	1	0
All	All	5285	0	4904	27	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 3.

All (27) 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:107:LEU:HD23	1:B:158:VAL:HG11	1.76	0.67
1:B:40:LEU:HD13	2:B:401:ECH:H33B	1.81	0.63
1:A:107:LEU:HD23	1:A:158:VAL:HG11	1.82	0.60
1:A:272:ARG:HH21	1:A:272:ARG:HG2	1.68	0.57
1:B:18:ALA:HB3	1:B:21:ILE:HD12	1.89	0.55
1:B:59:ALA:HB1	1:B:62:ILE:HB	1.88	0.54
2:B:401:ECH:H33	2:B:401:ECH:C8	2.38	0.54
1:B:73[B]:GLN:NE2	4:B:506:HOH:O	2.43	0.51
1:B:46:GLU:OE2	1:B:143:ARG:NE	2.44	0.49
1:A:287:ALA:HB2	1:A:306:LEU:HD21	1.94	0.49
1:A:46:GLU:OE2	1:A:143:ARG:NE	2.46	0.48
1:B:193:ILE:HD11	1:B:256:VAL:C	2.35	0.47
2:A:401:ECH:C8	2:A:401:ECH:H33	2.45	0.47
1:B:59:ALA:O	1:B:62:ILE:HG22	2.15	0.46
1:A:110:TRP:CD2	2:A:401:ECH:H33A	2.50	0.46
1:A:214:VAL:HG21	1:A:238:LEU:HB2	1.98	0.46
1:A:231:ILE:CD1	1:A:240:TYR:CD2	3.00	0.45
1:B:287:ALA:HB2	1:B:306:LEU:HD21	1.98	0.45
1:A:193:ILE:HD11	1:A:256:VAL:C	2.37	0.44
1:B:137:ASP:HA	1:B:140[A]:GLU:HG2	2.01	0.43
1:A:314:ASN:C	1:A:314:ASN:HD22	2.20	0.43
1:A:54:ALA:HB1	1:B:53:PRO:CD	2.49	0.42
2:B:401:ECH:C23	2:B:401:ECH:H40B	2.48	0.42
1:B:272[B]:ARG:HA	1:B:284:LEU:O	2.19	0.42
2:A:401:ECH:C23	2:A:401:ECH:H40B	2.50	0.42
1:B:17:VAL:HG12	1:B:304:ASP:HB3	2.02	0.42
1:A:260:ALA:HB2	1:A:266:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	315/321 (98%)	300 (95%)	14 (4%)	1 (0%)	41	46
1	B	325/321 (101%)	312 (96%)	9 (3%)	4 (1%)	13	10
All	All	640/642 (100%)	612 (96%)	23 (4%)	5 (1%)	19	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	PRO
1	B	57	SER
1	B	168	GLY
1	B	54	ALA
1	A	280	ASP

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	263/268 (98%)	250 (95%)	13 (5%)	25	31
1	B	267/268 (100%)	254 (95%)	13 (5%)	25	31
All	All	530/536 (99%)	504 (95%)	26 (5%)	28	31

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

Mol	Chain	Res	Type
1	A	69	ASN
1	A	136	SER
1	A	155	ARG
1	A	164	VAL
1	A	171	LYS
1	A	174	GLU
1	A	195	ASN
1	A	211	GLN
1	A	219[A]	GLU
1	A	219[B]	GLU
1	A	272	ARG

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Mol	Chain	Res	Type
1	A	310	LYS
1	A	314	ASN
1	B	1	MET
1	B	6[A]	ASP
1	B	6[B]	ASP
1	B	57	SER
1	B	70	GLU
1	B	73[A]	GLN
1	B	73[B]	GLN
1	B	77	LEU
1	B	136	SER
1	B	155	ARG
1	B	164	VAL
1	B	281	ASN
1	B	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	195	ASN
1	A	314	ASN
1	B	195	ASN
1	B	242	ASN
1	B	281	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	ACT	A	402	-	3,3,3	0.93	0	3,3,3	0.86	0
2	ECH	B	401	-	42,42,42	2.13	12 (28%)	55,58,58	1.82	16 (29%)
2	ECH	A	401	-	42,42,42	1.87	10 (23%)	55,58,58	2.03	14 (25%)

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
2	ECH	B	401	-	-	4/29/66/66	0/2/2/2
2	ECH	A	401	-	-	4/29/66/66	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ECH	C14-C13	6.95	1.45	1.35
2	A	401	ECH	C17-C18	6.47	1.44	1.35
2	B	401	ECH	C17-C18	5.39	1.42	1.35
2	A	401	ECH	C10-C9	4.10	1.41	1.35
2	B	401	ECH	C12-C13	-3.97	1.37	1.45
2	B	401	ECH	C23-C22	-3.92	1.37	1.45
2	B	401	ECH	C19-C18	-3.80	1.37	1.45
2	A	401	ECH	C19-C18	-3.51	1.38	1.45
2	B	401	ECH	C10-C9	3.45	1.40	1.35
2	A	401	ECH	C20-C21	-3.02	1.34	1.43
2	A	401	ECH	C23-C22	-2.95	1.39	1.45
2	A	401	ECH	C21-C22	2.83	1.39	1.35
2	B	401	ECH	C21-C22	2.72	1.39	1.35
2	A	401	ECH	C11-C12	2.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ECH	O27-C27	2.59	1.28	1.23
2	B	401	ECH	C25-C26	2.58	1.39	1.35
2	A	401	ECH	C8-C9	-2.48	1.40	1.45
2	A	401	ECH	C37-C22	2.45	1.55	1.50
2	B	401	ECH	C20-C19	2.35	1.40	1.34
2	B	401	ECH	C20-C21	-2.34	1.36	1.43
2	A	401	ECH	C14-C13	2.33	1.38	1.35
2	B	401	ECH	C34-C9	-2.28	1.46	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ECH	C15-C16-C17	5.43	134.60	123.47
2	B	401	ECH	C37-C22-C23	4.77	125.60	118.08
2	B	401	ECH	C15-C16-C17	4.65	133.01	123.47
2	A	401	ECH	C37-C22-C23	4.31	124.86	118.08
2	A	401	ECH	C11-C10-C9	4.00	133.02	127.31
2	B	401	ECH	C37-C22-C21	-3.93	117.42	122.92
2	A	401	ECH	C28-C27-C26	3.87	122.22	118.65
2	A	401	ECH	O27-C27-C28	-3.69	114.82	120.86
2	A	401	ECH	C34-C9-C10	-3.66	117.80	122.92
2	A	401	ECH	C20-C21-C22	3.47	132.26	127.31
2	A	401	ECH	C34-C9-C8	3.45	123.51	118.08
2	A	401	ECH	C37-C22-C21	-3.33	118.26	122.92
2	A	401	ECH	C29-C30-C25	3.26	115.50	110.48
2	B	401	ECH	C34-C9-C10	-3.16	118.49	122.92
2	B	401	ECH	C29-C28-C27	2.92	118.09	112.85
2	B	401	ECH	C24-C23-C22	-2.79	122.02	126.23
2	B	401	ECH	C16-C15-C14	2.76	129.12	123.47
2	A	401	ECH	C35-C13-C14	-2.62	119.25	122.92
2	B	401	ECH	C40-C30-C25	2.59	114.50	110.30
2	B	401	ECH	C11-C10-C9	2.58	131.00	127.31
2	A	401	ECH	C40-C30-C25	2.57	114.47	110.30
2	A	401	ECH	C30-C25-C24	2.49	122.83	115.78
2	B	401	ECH	C36-C18-C17	-2.49	119.44	122.92
2	B	401	ECH	C19-C18-C17	2.29	122.45	118.94
2	B	401	ECH	C30-C25-C24	2.29	122.25	115.78
2	B	401	ECH	O27-C27-C28	-2.24	117.18	120.86
2	A	401	ECH	O27-C27-C26	2.21	122.92	120.96
2	B	401	ECH	C29-C30-C25	2.16	113.80	110.48
2	B	401	ECH	C10-C11-C12	2.13	129.85	123.22
2	B	401	ECH	C28-C27-C26	2.04	120.53	118.65

There are no chirality outliers.
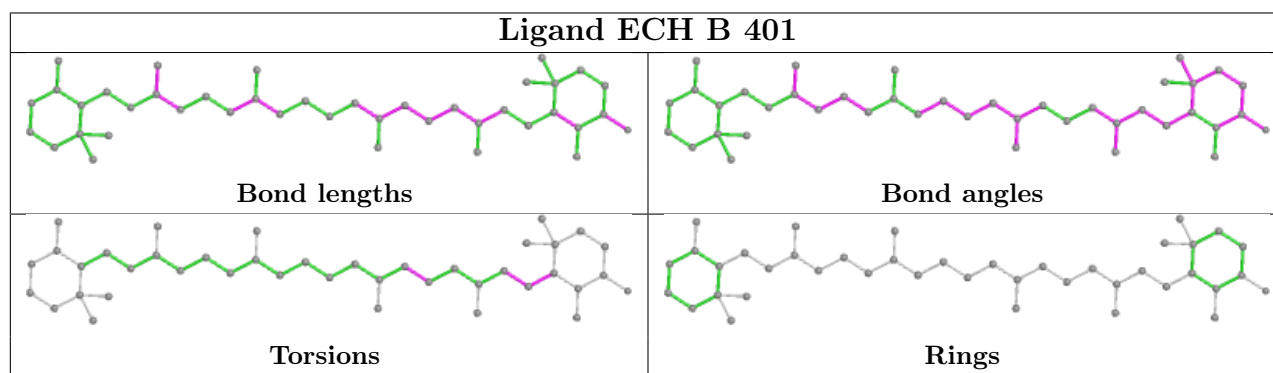
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ECH	C22-C23-C24-C25
2	B	401	ECH	C22-C23-C24-C25
2	B	401	ECH	C18-C19-C20-C21
2	A	401	ECH	C23-C24-C25-C26
2	A	401	ECH	C23-C24-C25-C30
2	B	401	ECH	C23-C24-C25-C26
2	B	401	ECH	C23-C24-C25-C30
2	A	401	ECH	C16-C17-C18-C36

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ECH	3	0
2	A	401	ECH	3	0

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 ECH B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ECH A 401

Bond lengths

Bond angles

Torsions

Rings
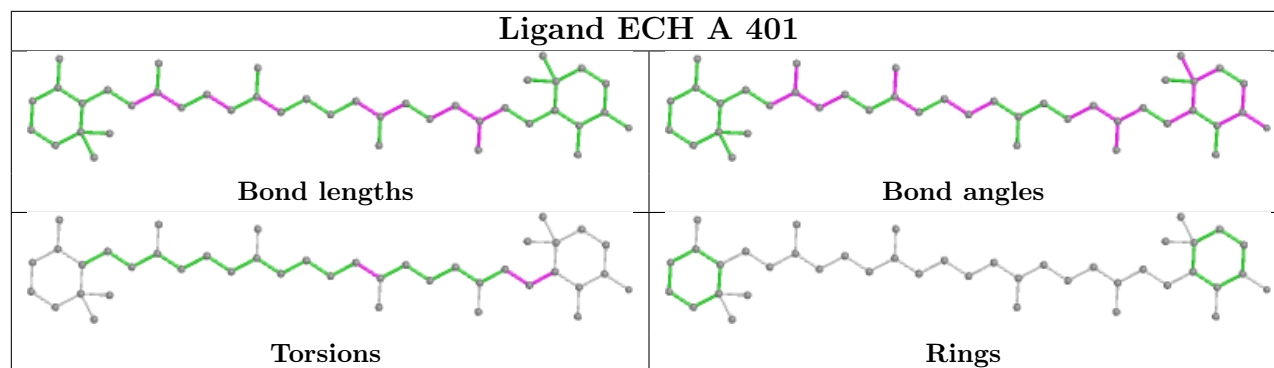
5.7 Other polymers ⓘ

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 ⓘ

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	314/321 (97%)	-0.53	2 (0%)	89 88	9, 17, 34, 54	0
1	B	319/321 (99%)	-0.32	8 (2%)	57 55	10, 19, 45, 82	0
All	All	633/642 (98%)	-0.43	10 (1%)	72 70	9, 18, 39, 82	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ALA	7.5
1	B	317	LEU	4.1
1	B	55	ALA	3.4
1	A	-1	SER	3.1
1	B	172	VAL	2.7
1	B	-1	SER	2.7
1	A	280	ASP	2.7
1	B	58	ALA	2.6
1	B	0	HIS	2.2
1	B	175	PRO	2.1

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

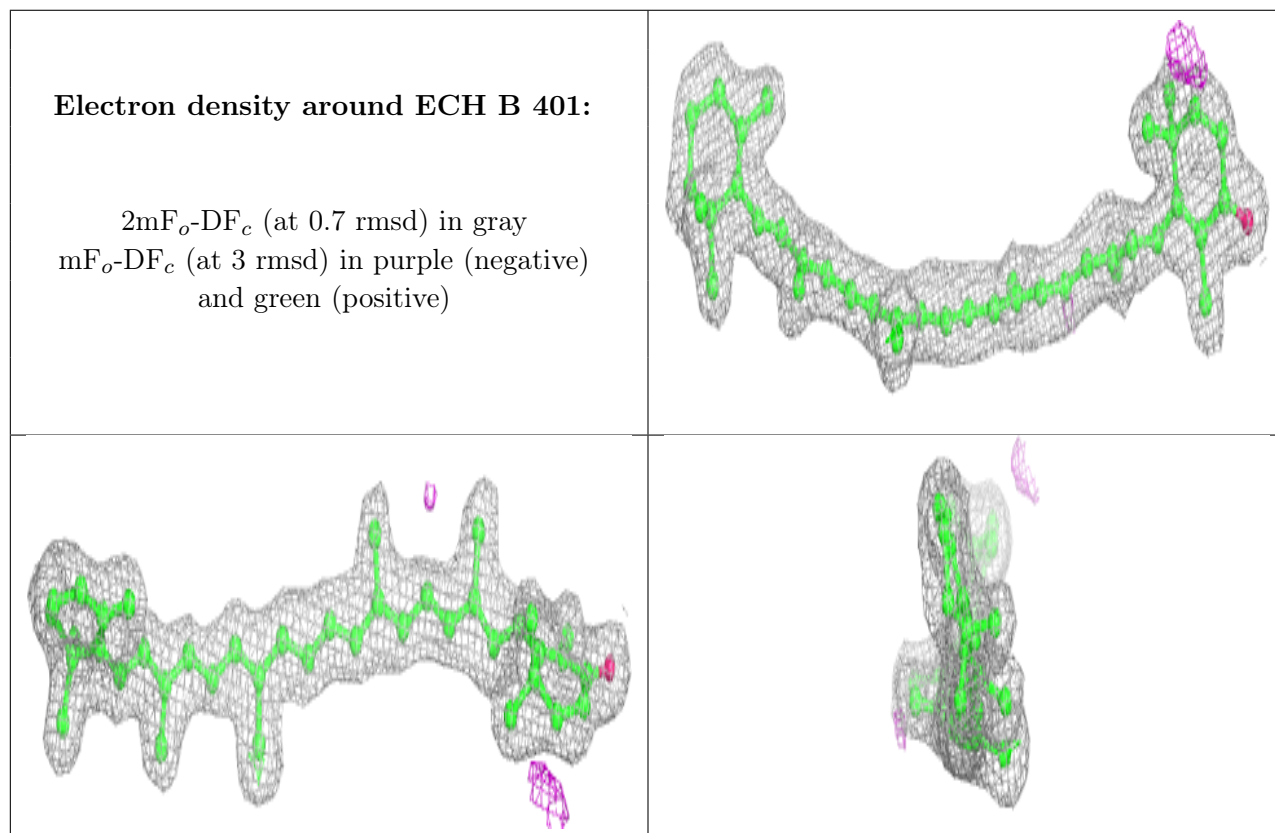There are no non-standard protein/DNA/RNA residues in this entry.

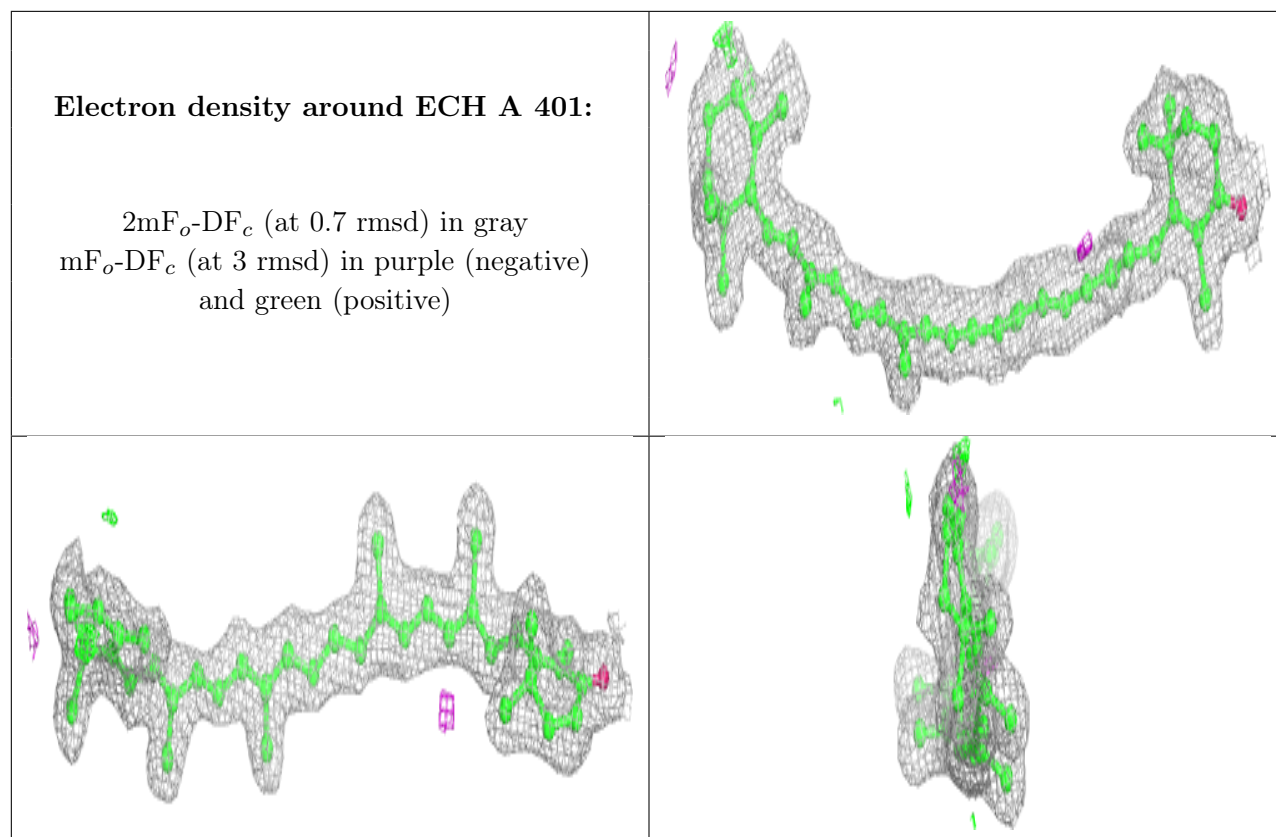## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	ACT	A	402	4/4	0.92	0.10	35,36,38,40	0
2	ECH	B	401	41/41	0.95	0.10	9,11,14,16	0
2	ECH	A	401	41/41	0.95	0.10	9,11,15,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ECH B 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around ECH A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.